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TRS-80 in-Stack Opacity Computer Programs
User and Programmer Manual

Atmospheric Research Group, Altadena, CA

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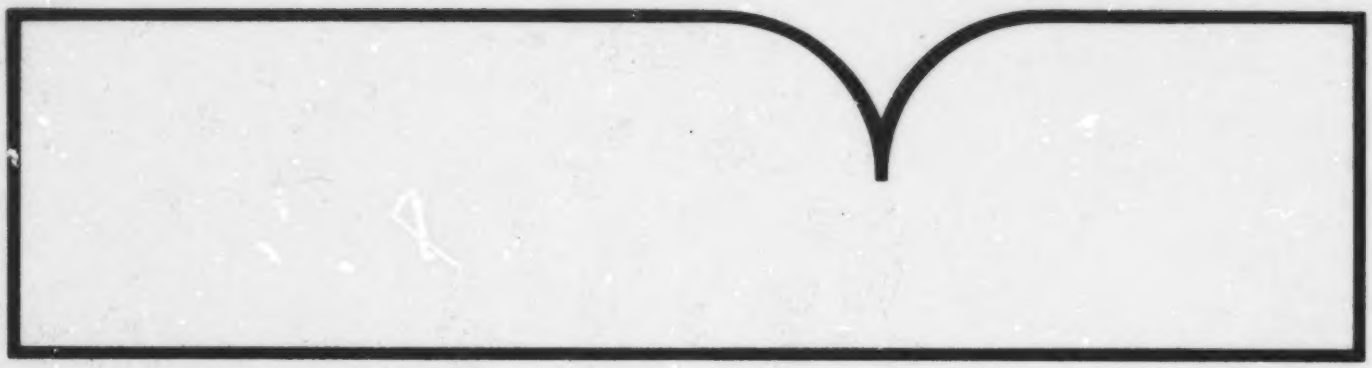

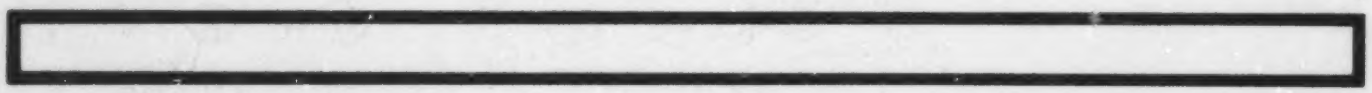

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TRS-80 IN-STACK OPACITY COMPUTER PROGRAMS: User and Programmer Manual

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16. ABSTRACT The manual describes a microcomputer program written to estimate in-stack opacity from ducted sources. Input data required to run the program are the particle size distribution, particle refractive index, mass emission concentration, wavelength of light, particle density, and stack diameter. The particle size distribution may be entered either as a histogram of particle diameter and fraction-greater-than-stated diameter or as log normal particle size distribution. The program calculates and displays the in-stack opacity. The program is written in the BASIC computer language and is specifically designed for the TRS-80 Model I, II, and IV computers. A moderate effort will be required to convert the programs to the IBM-PC and similar computers.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Pollution	Pollution Control	13B
Opacity	Stationary Sources	14G
Flue Gases	Particulate	21B
Estimating		
Computer Programs		09B
Particles		

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ABSTRACT

Computer programs were developed to predict in-stack opacity on a TRS-80 Model I, III, IV series of microcomputers. The programs are written in BASIC and use a "menu" format to input data.

The manual describes two different opacity programs: (1) a lognormal opacity program with particle size data in a lognormal format, and (2) a histogram opacity program with particle size data in a cumulative mass fraction versus particle diameter format. The light extinction properties of particles were calculated by using Mie equations in both programs. A Romberg integration routine is used in the lognormal opacity program, and a trapezoid integration and spline fit of particle size data are used in the histogram opacity program.

This manual presents operation of the programs, theoretical analysis of in-stack opacity, and a programmer's guide to changing or adapting the programs.

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SECTION 1

INTRODUCTION

SCOPE

This manual contains documentation for operating, understanding, and using in-stack opacity computer programs designed to run on a Radio Shack Model 1 TRS-80 microcomputer. The manual is divided into three sections: a user's guide to operation (Section 2), in-stack opacity theory (Section 3), and a programmer's guide (Section 4). The program listings are in Appendixes A and B.

Section 2 provides only the basic information for operating the programs. Sample calculations illustrate the type of data required for running the model and indicate the opacity predictions expected from correct operating procedures. The section also briefly explains the applications of this in-stack opacity model to actual visible emissions measured by an in-stack transmissometer or integrating nephelometer.

Section 3 explains the theoretical basis of the programs. The opacity theory model is based on the solution to the Mie equations describing light scattering by dielectric spheres (Born and Wolf, 1959). The interpolation of particle size data by a spline-fitting routine and integration techniques is also fully discussed. An error analysis enables the user to estimate the quality of an opacity prediction.

Section 4 describes the internal workings of the programs so the user can modify or adapt them for use on other systems. It also includes block diagrams, variable definitions, and debugging recommendations.

SYSTEM REQUIREMENTS

The TRS-80 Model 1 microcomputer system must contain 32K bytes of central random access memory (RAM), disk Level 2 BASIC, and two or more diskette drives. Both programs have an option for printing output on a standard line printer. The program can be run using the BASIC interpreter

or it can be compiled using the Microsoft compiler available from Radio Shack for a faster computation. The user should consult the Microsoft BASIC compiler manual for compilation instructions.

SECTION 2

USER'S GUIDE

APPLICATIONS OF IN-STACK OPACITY PROGRAMS

Predicting in-stack opacity is essential to designing control devices to meet strict opacity limitations. These programs predict visible emission in the stack as measured by an optical monitor such as a transmissometer or integrating nephelometer. The data required to make this prediction include:

1. Particle size distribution
2. Particle index of refraction
3. Mass concentration
4. Particle-specific gravity
5. Stack diameter.

These programs can also be used to determine the effect on opacity of changing operating conditions or size of a particulate control device. Opacity can be modeled for any situation where the physical and optical properties of the emission aerosol can be measured or estimated.

The user has a choice of two opacity programs, depending on the particle size distribution: lognormal or histogram. The histogram program will provide a least-squares lognormal fit of the size data. This lognormal fit is for the user's information only and is not used by the histogram program to compute opacity.

LOGNORMAL OPACITY PROGRAM

The lognormal opacity program computes in-stack opacity for an emission aerosol with a lognormal particle size distribution. The data are entered using a "menu" format. When the program is run, a menu will be displayed on the screen after a series of instructions are displayed.

The prime reason for using the menu format for entering data is so the data can be checked and corrected easily. The data should always be checked for accuracy of entry before calculations are begun.

The menu will list on one page all the data required for running this program. An arrow or cursor will point to a line of information containing its current value, a description of the item, and the units assigned to the item. The datum is entered and the cursor automatically shifts down to the next item. Move the cursor by pressing the up arrow (↑) key or down arrow (↓) key. When all the items are entered correctly, simply press the asterisk (*) to start computing. (Remember to hold down the SHIFT key.)

NOTE: The lognormal particle size distribution is represented by two variables, the mass mean diameter and the geometric standard deviation. The geometric standard deviation is limited so that division by zero does not occur. If this variable is less than 1.3, the size distribution is assumed to be monodisperse.

OPERATING THE LOGNORMAL OPACITY PROGRAM

Install the TRS-80 in a convenient location and connect it to a suitable source of power, as described in Section 1 of the Radio Shack TRSDOS Reference Manual (1979). The convention in this manual for indicating that a given key must be pressed will be the capitalization of all letters and underlining. To begin operation, place the diskette containing the TRSDOS system in Drive No. 0 and the diskette containing OPACITY1 in Drive No. 1. When the system is reset, the display will appear something like this:

```
TRSDOS - DISK OPERATING SYSTEM - VER 2.3

DOS READY
```

If the program has been compiled, simply type OPACITY1 and press ENTER. The No. 1 Drive will run, and the screen will read as shown in Figure 1.

If the program has not been compiled, load the software (type BASIC and press ENTER). The 0 disk drive will whir and the screen will read:

```
HOW MANY FILES? _____
```

```
═══════════════════════════════════════════════════════════════

OPACITY PREDICTION PROGRAM

═══════════════════════════════════════════════════════════════


THIS PROGRAM WAS DEVELOPED BY
S. COWEN (METEOROLOGY RESEARCH, INC.)
D. ENSOR (RESEARCH TRIANGLE INSTITUTE)
L. SPARKS (ENVIRONMENTAL PROTECTION AGENCY)
EPA PROJECT OFFICER - L. SPARKS - COOPERATIVE AGREEMENT #R806718010
PRESS ANY KEY ONLY ONCE.  A PAUSE MAY BE
NOTICED WHILE DEFAULT VALUE IS BEING ENTERED.
```

Figure 1. First screen display when the program "OPACITY1" is run.

Respond by pressing ENTER. The screen will read:

MEMORY SIZE? _____

Respond by pressing ENTER. The screen will read:

RADIO SHACK DISK BASIC VERSION 2.2

READY

> _____

Type: RUN"OPACITY1/BAS:1. The system will load the program and display the screen shown in Figure 1. Then press any key one time only. If the program has been compiled, the response will be almost instantaneous. Otherwise, wait about 5 seconds for the OPACITY PROGRAM HELP ROUTINE (see Figure 2) to be displayed. This routine explains the use of the menu data entry system.

Read the displayed instructions. When you understand them, continue by pressing any key. The screen will display:

```
DO YOU WANT LINE PRINTER OUTPUT?  TYPE Y OR N.
```

Press Y if the line printer output is desired. N if not. If Y is pressed and the line printer is ready to print, the screen will display:

```
YOU MAY ENTER UP TO THREE LINES OF COMMENTS
ENTER COMMENTS AND PRESS ENTER AFTER EACH LINE
```

If the line printer option is chosen and the line printer is not ready, the program will not continue until the line printer is operational.

The following part of the program allows the entry of information describing pertinent facts of the opacity calculation such as the plant description, date when measurements were taken, plant opacity conditions,

OPACITY PROGRAM HELP ROUTINE

THIS PROGRAM WILL PREDICT THE OPACITY OF A PLUME OF PARTICULATE MATTER.

DATA ENTRY IS HANDLED BY FILLING IN THE DATA FORM DISPLAYED ON THE CRT. THE FIRST AND ONLY FORM ASKS FOR GENERAL DATA SUCH AS WAVELENGTH OF LIGHT, REFRACTIVE INDEX. EACH DATA ITEM IS ASKED FOR BY NAME AND WITH THE REQUIRED UNITS. MOVE THE FORM BY PRESSING THE ↑ AND ↓ ARROWS. AFTER ENTERING A DATA ITEM, PRESS ENTER TO COMPLETE DATA ENTRY. WHEN THE PAGE IS FILLED, PRESS * TO START CALCULATION.

PRESS ANY KEY ONE TIME ONLY TO CONTINUE.

Figure 2. Opacity program HELP ROUTINE.

or unusual circumstances that may affect opacity data. Press ENTER after entering each line. (If there are more than three lines of comments, type three lines on the screen before pressing ENTER for a total of nine lines. However, the command CLEAR 800 must be at line 30 in the program to reserve enough memory for string space.)

After comments are entered, the screen will display:

OPACITY DATA ENTRY PAGE 1

→ REAL PART OF INDEX OF REFRACTION	1.50
IMAGINARY PART OF INDEX OF REFRACTION	0.000 I
WAVELENGTH OF LIGHT	0.55 MICRONS
MASS CONCENTRATION	0.010 G/M^3
PARTICLE DENSITY	2.4 G/CC
STACK DIAMETER	6.9 METERS
MASS MEAN DIAMETER	1.000 MICRONS
GEOMETRIC STD DEVIATION	2.000

↑↓ ARE ACTIVE.

USE * TO INITIATE CALCULATIONS. USE H FOR HELP.

This data entry page is used to input all the data required to run the lognormal opacity program. The data shown are default values to be used for the sample calculation. Enter a few items to become familiar with the menu operation. Simply type a number and press ENTER. That number will be the value of the variable designated by the arrow (→). After practicing data entry long enough to be comfortable with it, enter data as shown previously for the sample calculation. If problems arise, press H to obtain the HELP ROUTINE shown in Figure 2. This HELP ROUTINE can be

accessed only from data entry page 1. When all the data items have been checked, press * to begin calculation. (Remember to hold down SHIFT.)

First, the input data are printed on the line printer if that option is chosen. If the printer is not ready for operation, the program will not run! The screen will show the progress of the calculations; the opacity result should appear after about 6 minutes for the compiled version or about 46 minutes for the program run by the interpreter.

The first item printed on the screen will be:

"1 LOWER-UPPER DIAM .01 TO 0.1" .

This is the first range of the Romberg integration. (Details of the theory of the integration are discussed fully in Section 3. Debugging procedures are outlined in Section 4, Programmer's Guide.) The screen will print the values of three variables throughout the calculations: DIAM (particle diameter), Q (light extinction efficiency), and N(DP) (particle number distribution). When the particle diameter is greater than 7 μm; the light extinction efficiency is set equal to 2.0, the limiting value for large particles. These constant values are not printed out. After the integration is complete for a given range of particle sizes, a summary of values is printed: extinction (m^2/cm^3), volume distribution, number distribution, and the number of terms required for the Romberg integration to meet the integral tolerance of 0.01.

The light extinction is integrated over four decades of particle sizes from 0.01 to 100 μm. After completion of the integration, the following result will appear:

SPECIFIC EXTINCTION COEFFICIENT (m^2/cm^3) = 5.01098
OPACITY (%) = 13.4169

If these results do not appear, check data entry for correct values. If input data are correct, consult debugging procedures in Section 4.

HISTOGRAM OPACITY PROGRAM

This program computes in-stack opacity for an emission aerosol with any measured particle size distribution, lognormal or otherwise. The main advantages of this program over the lognormal program are:

1. Any measured particle size distribution can be used.
2. The contribution to opacity by a specific size range is provided.
3. This program will interpolate particle size measurements within the measurement size range and also extrapolate data outside the measured size range.

The main disadvantage of this program is its slower data entry and slower calculating time. Also the lognormal extrapolation outside the measured size range may not duplicate the actual particle size distributions.

The data entry for this program also involves using a "menu" format to facilitate operation. This menu contains from two to four pages of data entry depending on the number of particle sizes. The first page contains general information similar to the lognormal program, including particle index of refraction, wavelength of light, mass concentration, particle density, and stack diameter. The following data entry pages are used for the particle size distribution input in the form of mass fractional cumulative less-than values with the maximum number of particle sizes equal to 27.

The identical keys used for the lognormal program manipulate the cursor up (↑) or down (↓). The same HELP ROUTINE is also obtained by pressing H. When data entry for an entire page is complete, press > to advance to the following pages. Press < to return to earlier pages to check data entry or to change the value of a variable. Again, calculations are initiated by pressing *.

OPERATING THE HISTOGRAM OPACITY PROGRAM

Instructions for preparing the TRS-80 to run the histogram opacity program are identical to those used for the lognormal opacity program.

Once the system is in BASIC (uncompiled version only) and the disk containing the program is in Drive No. 1, type:

RUN "OPACITY9/BAS:1

If running the compiled machine language version with system in TRSDOS, type the name of the program: OPACITY9. The system will load the program and display the screen as shown in Figure 1. Press any key one time, and the screen will display:

```
================================================================

DO YOU WANT TO RUN SAMPLE CALCULATION?  Y OR N.

================================================================
```

Press Y if you want to run a sample calculation to check out the program or practice program operation. Otherwise, press N. Press any key one time, and the opacity HELP ROUTINE (similar to Figure 2) will be displayed. The main difference between the two routines is the amount of data entry: only one page for the lognormal program, but two to four pages for the histogram program.

To continue, press any key only one time. The screen will display:

```
================================================================

THE REMAINING PAGES ARE USED FOR THE PARTICLE SIZE DISTRIBUTION.

     THE PARTICLE SIZE DISTRIBUTION MAY BE ENTERED ONLY AS
     PARTICLE DIAMETER AND CUMULATIVE LESS THAN.  CONTROL
     MOVEMENT AROUND THE PARTICLE SIZE DISTRIBUTION FORMS USING
     THE FOUR ARROWS.  TO CHANGE PAGES USE < OR >.  WHEN ALL
     DATA ARE ENTERED AND ARE CORRECT, PRESS * TO BEGIN CALCULA-
     TIONS.  PRESS ANY KEY TO CONTINUE.

================================================================
```

This part of the routine explains the entry of particle size data and use of the correct keys to manipulate the forms. Read the displayed instructions. When they are understood, press any key one time to continue. The screen will display:

```
DO YOU WANT LINE PRINTER OUTPUT?  TYPE Y OR N.
```

Press Y if line printer option is desired; N if not. If Y is pressed, the screen will display (otherwise, the screen will skip to opacity data entry page 1):

```
YOU MAY ENTER UP TO THREE LINES OF COMMENTS.
ENTER COMMENTS AND PRESS ENTER AFTER EACH LINE.
```

As earlier, enter comments describing pertinent facts. After comments are entered, the screen will display:

```
OPACITY DATA ENTER PAGE 1

→ REAL PART OF INDEX OF REFRACTION              1.50
  IMAGINARY PART OF INDEX OF REFRACTION         0.000 I
  WAVELENGTH OF LIGHT                           0.55 MICRONS
  MASS CONCENTRATION                            0.010 G/M3
  PARTICLE DENSITY                              2.4 G/CC
  STACK DIAMETER                                5.00 METERS

↑ ↓ ARE ACTIVE.  USE > TO GO TO NEXT PAGE.
USE * TO INITIATE CALCULATIONS.
USE H FOR HELP.
```

This data entry page is used to input general data for the opacity histogram program. The data shown are default values to be used for the sample calculation. The data entry procedure is similar to the menu format used by the lognormal program. The only difference is that > is used to advance the menu to following pages.

When all data items have been entered and checked, press > (remember to hold down SHIFT) to go to following pages. The screen will display:

```
ENTER PARTICLE SIZE DISTRIBUTION
AS A CUMULATIVE MASS
FRACTION LESS THAN.
START WITH SMALLEST PARTICLE DIAMETER.
THE CUMULATIVE MASS FRACTION MUST INCREASE
FROM SMALLEST TO LARGEST DIAMETERS!
PRESS ANY KEY TO CONTINUE.
```

The displayed instructions are a reminder of particle size data input procedures. Follow the displayed instructions strictly to obtain correct results. Read the displayed instructions. When they are understood, press any key to continue. The screen will display:

```
═══════════════════════════════════════════════════════

I.   DIAMETER MICRONS                CUMULATIVE MASS (<)

1        →.2                              .0101184
2         .4                              .0930961
3         .5                              .158655
4         .7                              .303426
5        1                                .5
6        1.5                              .720713
7        2                                .841345
8        2.5                              .906904
9        4                                .97725

═══════════════════════════════════════════════════════

↑ ↓ → ←ARE ACTIVE.  USE * TO START CALCULATIONS.

USE > TO GO TO NEXT PAGE, < TO GO TO PREVIOUS PAGE.
```

This data entry page shows default values for the cumulative mass less than particle size data for the first nine diameters. The form manipulation symbols are identical to those of the previous operation. The arrows control the position of the cursor on the page. The > and < control data entry page movement. The * starts calculations. After a particle diameter is entered, the cursor will automatically progress from left to right across the page. If a cumulative mass fraction is entered, the cursor will move down to the following particle diameter.

Press ≥ to advance to the next page, and the screen will display:

I.	DIAMETER MICRONS	CUMULATIVE MASS (<)
10	→7	.997504
11	10	.999555
12	0	0
13	0	0
14	0	0
15	0	0
16	0	0
17	0	0
18	0	0

↑ ↓ , →ARE ACTIVE. USE * TO START CALCULATIONS.

USE > TO GO TO NEXT PAGE, < TO GO TO PREVIOUS PAGE.

This data entry shows particle size data for 10th through 18th particle diameters. The default case shows only 11 data points and thus zeros are indicated for the 12th through 18th points. If ≥ is pressed, size data for the 19th through 27th particle diameters can be entered. These values also equal zero for the default case. A maximum of 27 points can be entered.

NOTE: The particle diameter required by this program is the physical diameter. Conversion of an aerodynamic diameter to the physical diameter is discussed in Section 3.

Run the sample collection by pressing the asterisk (*) key. First the input data are printed on the line printer if that option is chosen. The printer must be ready for operation or the program will not run. The screen will show the progress of the calculations and the opacity results should appear after approximately 7 minutes for the compiled version and approximately 65 minutes for the program run by the BASIC interpreter.

The next item shown by the printer and displayed on the CRT is a least-squares fit of the particle size data to a lognormal distribution. The values calculated for the sample calculation are:

```
MASS MEDIAN DIAMETER          =  .999956
GEOMETRIC STD DEV             = 1.99968
LOGNORMAL FIT PARAMETER       = 1
(CORRELATION COEFFICIENT)
```

The lognormal fit parameter represents the correlation coefficient of the particle size data to a lognormal distribution. A value of 1 indicates a perfect correlation; 0 indicates no correlation.

The screen will next display on the CRT the identical variables printed by the lognormal program:

```
LOWER - UPPER DIAMETER        .01 - .2
DIAM = .01     Q = 2.4522E-06
N(DP) = 6.65261E-04
```

These variables will continue to be displayed as the integration goes from 0.01 to 100 μm. The integral in the sample calculation has been divided into 12 parts. The first integration goes from 0.01 to the first diameter from the input size distribution; i.e., 0.2. The subsequent integrals integrate from the first diameter to the second diameter, the second to the third, etc.

The last integral in this sample is the integration from the last input diameter (i.e., 11th diameter, 10) to 100 μm. The following will be on the screen and printed out for each size increment, for example:

```
LOWER - UPPER DIAMETER   .01 - .2
EXTINCTION       VOLUME        NUMBER
2.103E-02      1.971E-02      6.807E+00
```

When the computation is complete, the following will be displayed on both the monitor and printer INTEGRALS (EXTINCTION, VOLUME, NUMBER)=

6.34833 1.91115 16.684

The percent contribution of a given particle size range to each of these integrals is computed. If more than 50 percent of the light extinction occurs outside the measured particle size range (in this sample calculation, measured size range is from 0.2 to 10 μm), a warning is printed stating that the opacity prediction is inaccurate because of insufficient data. The final output of the sample calculation should match exactly:

LOWER - UPPER DIAMETER		%EXTINCTION	%VOLUME	%NUMBER
.01	.2	.331233	1.03118	40.7893
.2	.4	10.418	8.3044	36.8844
.4	.5	11.9711	6.55583	8.3751
.5	.7	27.8496	14.4795	8.10212
.7	1	27.5338	19.626	3.97903
1	1.5	12.3447	22.0381	1.48577
1.5	2	5.52884	12.0658	.280904
2	2.5	2.108	6.55577	.0698805
2.5	4	1.60802	7.03324	.031266
4	7	.286712	2.0275	2.21946E-03
7	10	.0155717	.205113	4.79287E-05
10	100	4.56549E-03	.0776255	8.5245E-06
SPECIFIC EXTINCTION COEFFICIENT (m^2/cm^3) =				4.98299
OPACITY (%) = 9.86055				

If these results are not obtained, check data entry for correct values. If input data are correct, consult Section 4 for debugging procedures.

One potential problem with this program operation is the generation of a negative value of the number size distribution (physically impossible) by the extrapolation routine. A short message "NEGATIVE N(DP) @ DIAMETER = VALUE OF DP" will be displayed briefly on the CRT. The program sets these values equal to zero and proceeds with the calculation. The end results will not be greatly affected unless most of the light extinction occurs outside the measured particle size range. This can be checked by referring to the table output of percent extinction vs. particle size range.

SECTION 3

IN-STACK OPACITY THEORY

BACKGROUND

In-stack opacity refers only to opacity as measured by transmissometers in a stack. Out-of-stack plume opacity is much more complex and is beyond the scope of this work. An out-of-stack opacity measurement by observation requires understanding the effect of background contrast, light-scattering angles, and condensable material such as sulfuric acid. Out-of-stack opacity can also be measured by instrumental techniques such as lidar and photometry, which are less sensitive to environmental factors than observers. When condensables are present, plume opacity may be much greater than in-stack opacity because more light is scattered by increased aerosol concentration.

THEORETICAL SUMMARY

The transmission of light through a volume containing an aerosol is described by the Beer-Lambert law:

$$\text{Opacity} = 1 - \text{transmittance} = 1 - I/I_o = 1 - \exp(-B_e L) \qquad (1)$$

where

I = transmitted light,
I_o = incident light,
B_e = the light extinction coefficient, and
L = the illumination pathlength (generally stack diameter for our case).

Following the ideas of Ensor (1972), the aerosol mass concentration is related to optical transmittance through a modified form of the Beer-Lambert law:

$$\frac{I}{I_o} = \exp \frac{-ML\ S_v}{\rho} \qquad (2)$$

where

M = the particle mass concentration (actual conditions g/m^3),

S_v = the ratio of the light extinction coefficient to specific particulate volume (m^2/cm^3), and

ρ = the average particle density (g/cm^3).

The specific extinction coefficient, S_v, is defined mathematically as:

$$S_v = \frac{\frac{3}{2} \int_0^\infty d_p^2 Q(d_p, \lambda, m)(d_p) d\, d_p}{\int_0^\infty d_p\, {}^3 n(d_p) d\, d_p} \qquad (3)$$

where

d_p = the particle diameter (μm),

$Q(d_p, \lambda, m)$ = the light extinction efficiency factor,

λ = the wavelength of incident light,

m = the aerosol index of refraction, and

$n(d_p)$ = the number particle size distribution.

Thus, S_v is defined for a given particle size distribution, particle index of refraction, and wavelength of incident light, and is the indicator of light extinction properties of the aerosol mass.

In the original Ensor (1972) development, parameter K, the reciprocal of S_v, was defined. Parameter K was useful in relating transmittance to mass concentration by:

$$M = \ln(I/I_o) \frac{K\rho}{L} \quad . \qquad (4)$$

Calculations of parameter K as a function of particle geometric mass mean radius and geometric standard deviation are shown in Figures 3 and 4 for transparent and absorbing aerosols, respectively.

The light extinction efficiency, $Q(d_p, \lambda, m)$, is calculated by using the Mie equation for the particle size ranges associated with particulate control devices (0.01 to 100 μm diameters). Expressions for the scattering and extinction efficiencies are obtained by solving Maxwell's equations for the interaction of a plane wave with a homogeneous sphere. The complete derivation is explained by Born and Wolf (1959).

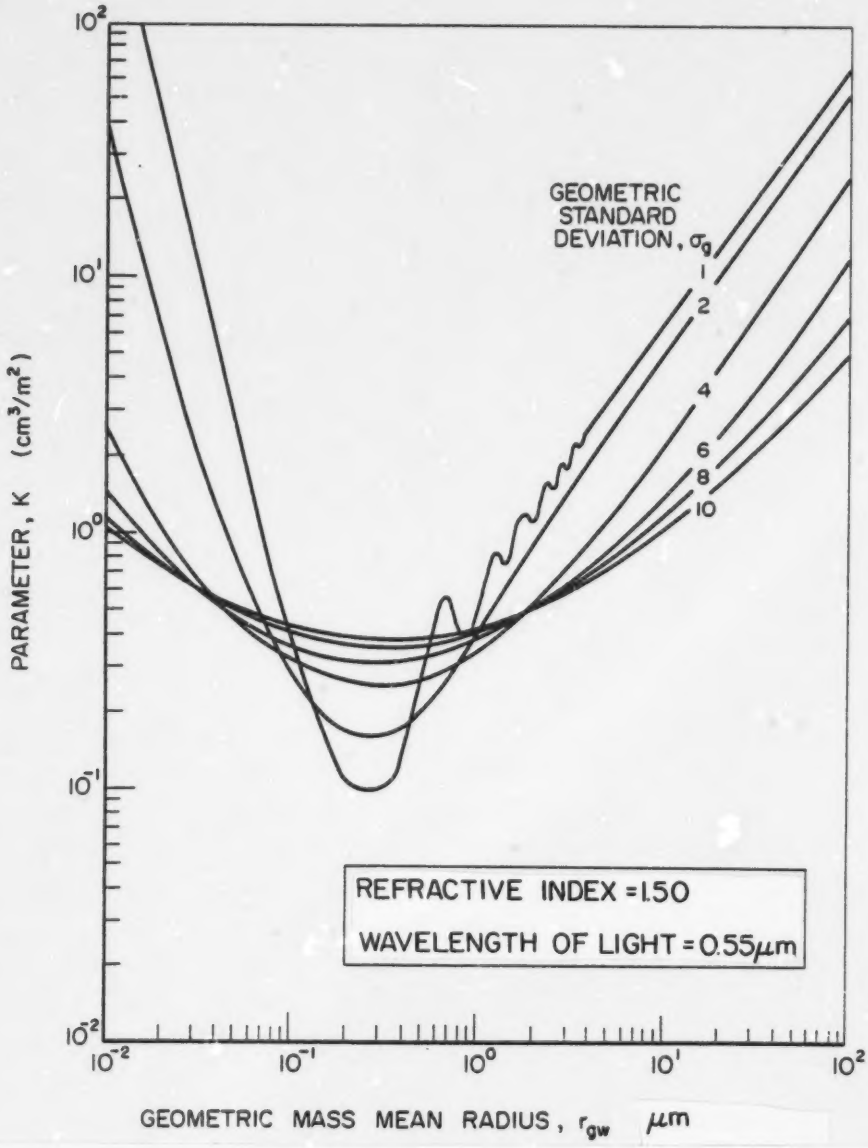

Figure 3. Parameter K as a function of particle size distribution for transparent aerosol.

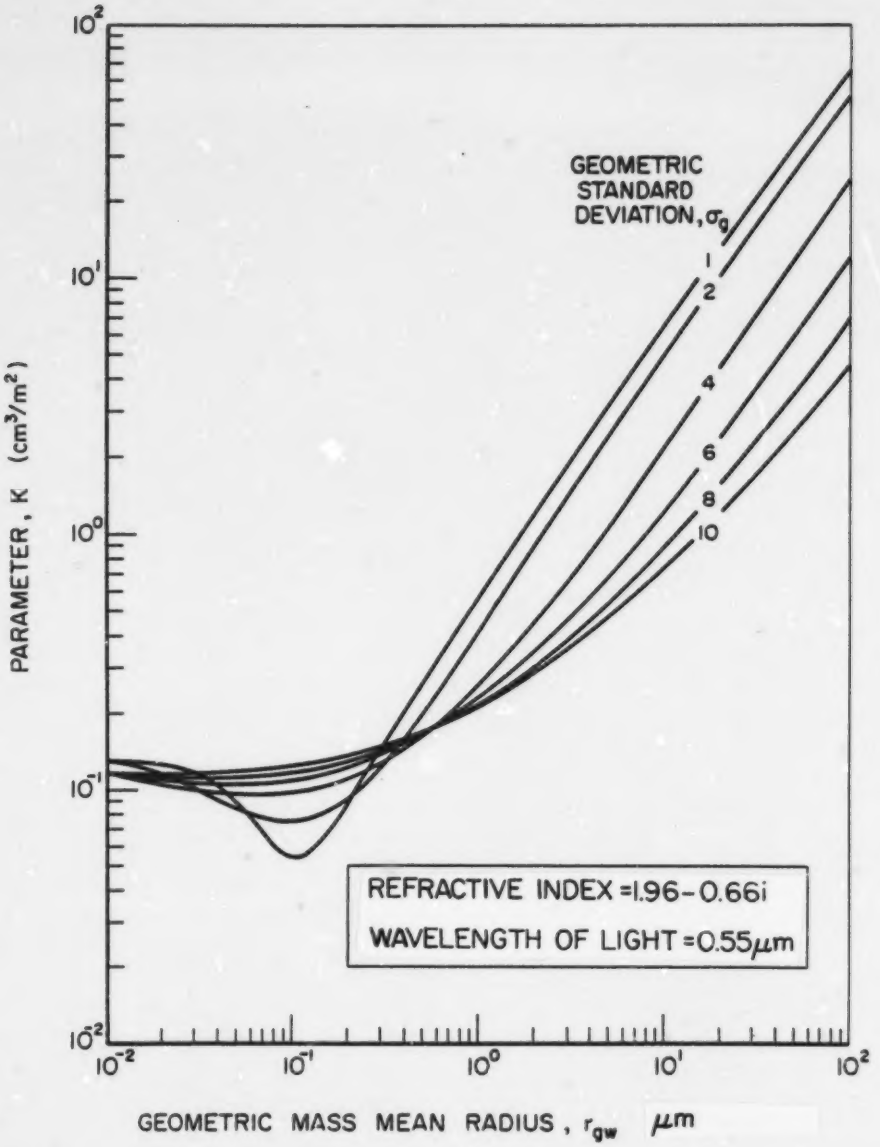

Figure 4. Parameter K as a function of particle size distribution for absorbing aerosol.

In-stack opacity is calculated by summarizing the above equations as:

$$\text{Opacity (\%)} = \left[1 - \exp -\left(\frac{S_v\ ML}{\rho}\right)\right] \times 100 \quad . \tag{5}$$

This assumes a constant particle density and index of refraction. Generally, a 0.55-μm wavelength of incident light is used as a representative of the maximum photopic response of the human eye.

MIE THEORY EXTINCTION EFFICIENCY

The Mie theory light extinction efficiency factor, a dimensionless quantity, is defined as the energy scattered and absorbed by the particle divided by the energy intercepted by the particle based on its geometric cross section. The extinction efficiency, as derived by van de Hulst (1957), is given by:

$$Q_{ex}\ (m,\ x) = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n + 1)\ \text{Re}\ \{a_n + b_n\} \tag{6}$$

where

m = the index of refraction, and

x = the size parameter $\frac{\pi d_p}{\lambda}$.

The Mie coefficients, a_n and b_n, are functions only of m and x, and Re indicates the real part of the bracketed term in Equation (6).

Deirmendjian (1969) adapted the Mie coefficients into a computational form by manipulating Bessel functions to obtain:

$$a_n(m,\ x) = \frac{\left[\frac{A_n(y)}{m} + \frac{n}{x}\right]\ \text{Re}\ \left[w_n\ (x)\right] - \text{Re}\ \left[w_{n-1}(x)\right]}{\left[\frac{A_n(y)}{m} + \frac{n}{x}\right]\ w_n(x) - w_{n-1}(x)} \tag{7}$$

and

$$b_n(m,\ x) = \frac{\left[m\ A_n\ (y) + \frac{n}{x}\right]\ \text{Re}\ \left[w_n(x)\right] - \text{Re}\ \left[w_{n-1}(x)\right]}{\left[m\ A_n(y) + \frac{n}{x}\right]\ w_n(x) - w_{n-1}(x)} \tag{8}$$

where

$$w_n(x) = \frac{2n-1}{x} w_{n-1}(x) - w_{n-2}(x),$$

$$w_0(x) = \sin x + i \cos x,$$

$$w_{-1}(x) = \cos x - i \sin x,$$

$$A_n(y) = -\frac{n}{y} + \left[\frac{n}{y} - A_{n-1}(y)\right]^{-1} \qquad y = m x \ , \tag{9}$$

and

$$A_0(y) = \frac{\sin p \cos p + i \sinh q \cosh q}{\sin^2 p + \sinh^2 q} \qquad \begin{matrix} p = n_1 x \\ q = n_2 x \end{matrix} \ . \tag{10}$$

These equations are then compacted by algebraic manipulations to reduce the number of computations and computing time.

The value of the refractive index for mineral material such as fly ash is roughly 1.5 with little absorption. The imaginary part of the complex refractive index determines the amount of light absorption. The results of the study of the optical properties of fly ash by Cowen et al. (1981) indicate a range of values of the refractive index from 1.53 to 1.61 for the real part (n_1) and from 0.0012 to 0.029 for the imaginary part (n_2).

The extinction efficiency for a refractive index of 1.5 is shown in Figure 5 as a function of the particle diameter. The curve goes through a series of maxima and minima: the maxima correspond to the reinforcement of transmitted and diffracted light, and the minima to light interference. The extinction efficiency approaches a value of 2 for large values of x. This factor is used in the opacity program for quick calculation of large particle scattering. The extinction calculation is the most time consuming calculation in the program, and the larger the particle size the more iterations are required.

LOGNORMAL OPACITY PROGRAM THEORY

This program computes opacity for lognormal particle size distributions. The usefulness of the program is that many of the aerosol emissions from coal-fired boilers have been measured and fit this functional form well. This program is especially useful for making in-stack opacity predictions

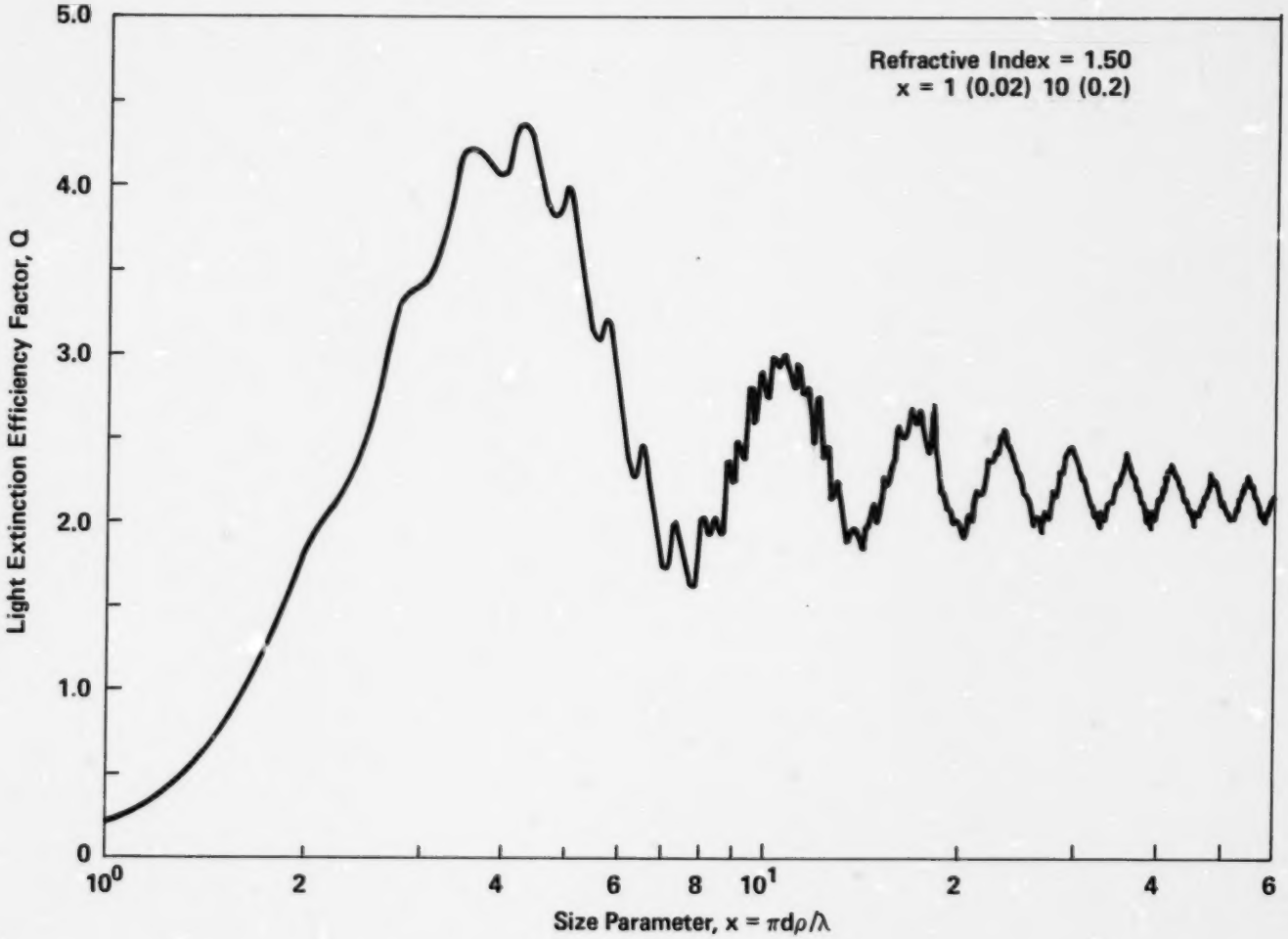

Figure 5. Light extinction efficiency as a function of size parameter.

for new installations where measurements of physical and optical properties of the aerosol emissions are not available. However, if these data can be obtained and the particle size measurements are not in a lognormal distribution, then the "histogram" opacity program should be used.

The histogram opacity program will output a least-squares lognormal fit of the size data, providing the user with the closest mass mean diameter, geometric standard deviation, and correlation coefficient. If this correlation coefficient is greater than 0.98, the outputs from the two programs will be similar.

The following comparison is an example of this similarity:

	Histogram Program	Lognormal Program
Mass mean diameter (μm)	= 1.376	1.376
Geometric standard deviation	= 2.194	2.194
Lognormal fit parameter	= 0.98	--
Specific extinction coefficient (m^2/cm^3)	= 3.04	3.84
Opacity (%)	= 35.7	44.8

Lognormal Size Distribution

The lognormal opacity program computes in-stack opacity for an aerosol mass with a lognormal particle size distribution. This size distribution is represented by:

$$f(d_p) = \frac{1}{\sqrt{2\pi} \ln \sigma_g \, d_p} \exp \frac{-\ln^2(d_p/d_g)}{2 \ln^2 \sigma_g} \qquad (11)$$

where

d_p = the particle diameter,

σ_g = the geometric standard deviation, and

d_g = the geometric mass mean diameter.

This mass size distribution, $f(d_p)$, must be converted to the number distribution, $n(d_p)$, required by the integral in Equation (3) to calculate the specific extinction coefficient, S_v. The geometric mass mean diameter is converted to the number mean diameter by the relationship:

$$\ln D_o = \ln (d_g/_2) - 3 \ln^2 \sigma_g \qquad (12)$$

where

D_o = the number mean diameter.

Romberg Integration

The integration is performed in four parts using a Romberg routine over four orders of magnitude from 0.01 to 100 μm. The derivation of the Romberg integration is described in detail by Ralston and Wilf (1967). The Romberg routine is an adaptive quadrature that automatically determines the integration interval to meet a prescribed accuracy requirement. The fractional error tolerance for this opacity program equals 0.01. However, this value can easily be changed if greater accuracy is desired. Refer to Section 4, Programmer's Guide, for instructions regarding this change.

In the Romberg integration, the trapezoid rule is applied first by calculating the function at the endpoints of range of the integral and its midpoint. Then a table of values of $F_a^{(b)}$ (approximations to the integral) is calculated by the Romberg difference algorithm given by:

$$F_a^{(b)} = \frac{4^a F_{a-1}^{(b+1)} - F_{a-1}^{(b)}}{4^a - 1} \qquad \begin{matrix} a = 1,2,... \\ b = 0,1,2,,... \end{matrix} \qquad (13)$$

This value of $F_a^{(b)}$ is the sum computed in the trapezoidal rule with 2^b subintervals. Then the value of $F_a^{(o)}$ is compared to that of $F_{a+1}^{(o)}$, and the tolerance is calculated. If this value is greater than 0.01, the interval is halved and the Romberg difference algorithm is used again to calculate new values of $F_a^{(b)}$. The process is repeated until the tolerance is obtained.

HISTOGRAM OPACITY PROGRAM THEORY

This program computes opacity for any real particle size distribution by performing two main manipulations of the particle size data. The first change involves a lognormal transformation. The second manipulation involves fitting the particle size data to a smooth spline function. The interpolation between measured particle sizes and extrapolation beyond the measured size range are performed by forcing the data along a curve represented by a natural spline. The result is a near-perfect match between the histogram and lognormal programs of a lognormal particle size distribution. However,

a particle size distribution that deviates from a lognormal fit (especially at the upper and lower boundaries of the measurement range) will extrapolate into a negative number distribution. This physically impossible situation was not remedied by application of an unnatural spline. These negative values are set equal to zero in the program to avoid artificial bias. This extrapolation difficulty is not serious because the particle mass outside the measured range is normally small; its light extinction properties are also relatively insignificant.

Method of Integration

The integration of this program applies to a simple trapezoidal rule for particle diameters from 0.01 to 100 μm. The Romberg integration was attempted; but correct results could not be obtained independent of the integration tolerance. The integration depends on the particle size data entered by the user. The order of integration is:

1. The first integral includes the particle size range from 0.01 μm to the first diameter of the input particle size data.

2. Integrals are computed for each interval in the input particle size data.

3. The last integral computes from the last diameter of the input particle size data to 100 μm.

Each integral part is divided into 10 equal intervals for the trapezoid calculation. Also, each integral is printed along with the fractional contribution of that integral to total light extinction, volume, and number size distributions.

Lognormal Transformation

A lognormal transformation of the particle size data is performed according to the procedure outlined by Lawless (1981). This transformation allows an exact fit of interpolation techniques to a lognormal distribution. The basis of this transformation relates to the measured lognormal particle size distributions emitted from combustion sources. The transformation is achieved by computing the logarithm of the particle diameter and the normal transform of the cumulative mass functions.

The cumulative function F is given by:

$$F(y) = \int_{-\infty}^{y} \frac{e^{-t^2/2}}{\sqrt{2\pi}}\, dt \qquad (14)$$

when

y = log (particle diameter).

The normal transformation, N_1, is the inverse function of F but is not analytic. It can be approximated by the polynomial expression:

$$-Q(F) = -x = t - \frac{C_0 + C_1 t + C_2 t^2}{1 + d_1 t + d_2 t^2 + d_3 t^3} \qquad (15)$$

where

$$t = \sqrt{\log\left(\frac{1}{F^2}\right)} \quad 0 \leq F \leq 0.5$$

and

$C_0 = 2.515517$,
$C_1 = 0.802853$,
$C_2 = 0.010328$,
$d_1 = 1.432788$,
$d_2 = 0.189269$, and
$d_3 = 0.001308$.

This expression is valid only for F from 0 to 0.5. Hence the following relation is required to complete calculations for F from 0.5 to 1.0:

$$F(-x) = 1 - F(x) \; . \qquad (16)$$

The derivative of the cumulative function is proportional to dm/dlogD, or the differential size distribution. Since the differential size distribution is required, the transformed cumulative function must be changed back to linear space by using the relation:

$$yy = Q(F(n)) \; . \qquad (17)$$

The derivative of the cumulative function mathematically follows from this relation:

$$F'(x) = \exp(-yy^2(x)/2) \cdot Y1(x) \qquad (18)$$

where

yy = the normal transformation of the cumulative function and Y1 is its derivative.

If Y1 is constant, the particle size distribution is normally distributed.

Spline Interpolation

Spline interpolation is used in the histogram program because spline interpolation is generally the best procedure for differentiating tabular data.

The spline function is a type of polynomial curve that passes through all the data points and has continuous first and second derivatives. The spline is made to conform to data points by means of weighted pivots. The spline interpolation used by the histogram opacity program is a third-order natural spline consisting of a cubic polynomial passing through the data points with the second derivative at the first and last data points equal to zero. Application of the spline function to cascade impactor data is described by Lawless (1981). The equation of this spline function is given by:

$$S(x) = y_i + b_i (x-x_i) + C_i (x-x_i)^2 + d_i (x-x_i)^3, \text{ for } x_i \leq x \leq x_{i+1} . \qquad (19)$$

The characteristic of this spline that forces the curve exactly through the data points may tend to produce unrealistic results (i.e., negative numbers) when extrapolating outside the data. However, its interpolating properties are quite adequate since it is relatively insensitive to changes in a single data point. Thus, an error in the data does not propagate throughout the particle size range. Also, any error in the extrapolation is mitigated by the relatively small light extinction normally occurring in those regions.

The third-order natural spline is calculated from the following tri-diagonal set of equations for the spline second derivatives $S''(X_k)$:

for

$$H_k = X_k - X_{k-1} \qquad k = 2,\ldots N \tag{20}$$

$$\frac{H_k}{6} S''(X_{k-1}) + \frac{H_k + H_{k+1}}{3} S''(X_k) + \frac{H_{k+1}}{6} S''(X_{k+1}) =$$

$$\frac{F(X_{k+1}) - F(X_k)}{H_{k+1}} - \frac{F(X_k) - F(X_{k-1})}{H_k}$$

with

$$S''(X_1) = S''(X_n) = 0 \quad . \tag{21}$$

A successive overrelaxation technique is used to solve these equations for the interior second derivative, repeated until the residual is less than 1×10^{-6}. After the third derivatives are calculated using finite approximations with difference equations, the values of the spline and its derivatives at the data points are used to interpolate and extrapolate required particle sizes. The extrapolation utilizes the first derivatives at the end data points to compute the normal transformation of the cumulative mass function and its derivative. This computation is described by:

$$Y1(X) = \frac{y_{i+1} - y_i}{X_{i+1} - X_i} - \frac{(X_{i+1} - X_i) \cdot 2 \cdot \left[\frac{y_{i+2} - y_{i+1}}{X_{i+2} - X_{i+1}} - \frac{y_{i+1} - y_i}{X_{i+1} - X_i}\right]}{(X_{i+1} - X_i) + (X_{i+2} - X_{i+1})} \tag{22}$$

and

$$yy(X) = [y_i + (\log (d_p) - X_i)] \cdot Y1 \tag{23}$$

for

$i = 1$ when the equation is used to extrapolate from the lower limit the first data point

and

$i = N-1$ when the equation is used to extrapolate from the last data point to the upper limit

when

N = the number of data points, and

d_p = the particle diameter.

The interpolation between data points is accomplished by using the second and third derivatives of spline to calculate yy(X) and Y1(X):

$$yy(X) = y_i + (\log d_p - X_i) \cdot \frac{y_{i+1} - y_i}{X_{i+1} - X_i} + PR \cdot DQ \qquad (24)$$

where

$$PR = (\log d_p - X_i) \cdot (\log d_p - X_{i+1}) \qquad (25)$$

and

$$DQ = [2 \cdot S''(X_i) + S''(X_{i+1}) + (\log d_p - X_i) \cdot S''(X_i)] \div 6 \qquad (26)$$

then

$$Y1 = \frac{y_{i+1} - y_i}{X_{i+1} - X_i} + [(\log d_p - X_i) + (\log d_p - X_{i+1})] - DQ + PR \cdot S''(X_i) \div 6 \qquad (27)$$

for

i = 1 to N.

The divided differences are used to approximate the second and third derivatives. Forsythe et al. (1977) provide a more complete derivation.

Conversion of Aerodynamic Diameter to Physical Diameter

Aerosol size data are often reported in terms of the aerodynamic diameter, defined as the diameter of a hypothetical sphere of unit density with the same Stokes number as the particle in question. Particles of different size, shape, and density may have the same aerodynamic diameter.

The conversion of aerodynamic diameter to physical diameter is derived from the Stokes formulation:

$$St = \frac{\rho d_p^2 \, Uav}{C \, 18 \, \mu d_j} \qquad (28)$$

where

St = the nondimensional Stokes number,

ρ = the particle density,

d_p = the particle diameter,

Uav = the average impactor jet velocity,

C = the Cunningham slip correction factor,

μ = the viscosity, and

d_j = jet diameter.

For particles with physical diameters greater than 2 μm, the Cunningham correction factor is approximately 1 and the conversion is:

$$d_{p_{physical}} = \frac{d_{p_{aerodynamic}}}{\rho^{1/2}} . \quad (29)$$

The conversion for smaller diameters requires an iterative calculation because the correction factor is a function of particle diameter for small particles. The correction factor is empirically given by:

$$C = \frac{2\lambda}{d_p} (1.25 + 0.42e^{-0.87\, d_p/2\lambda})$$

where

λ = the mean free path.

The mean free path is calculated by:

$$\lambda = 0.131 \left(\frac{T_{stack}}{T_{std}}\right) \cdot \frac{P_{std}}{P} \quad (30)$$

where

T_{stack} = the stack temperature (K),

T_{std} = the standard temperature (294.1 K),

P_{std} = the standard pressure (1 atm), and

P = the impactor pressure (atm).

ERROR ANALYSIS

The user of these opacity prediction programs should understand the quality of the prediction or a rough estimate of the error bounds. This discussion focuses on two main areas concerning introduction of error into the opacity prediction:

1. Inherent errors in the programs caused by roundoff errors, numerical truncation, program approximations, and program limitations.

2. Sensitivity analysis of the opacity equation; i.e., the assessment of the relative importance of input parameters.

This error analysis attempts to resolve the major uncertainties in predicting opacity. Knowledge of the major causes of error is required to define the accuracy of an opacity prediction. The determination of this error may seem to be straightforward, consisting of quantifying the errors of the dependent parameters. However, this discussion shows that the largest error cannot be attributed to just one measured parameter. It must focus on a composite of two basic measurements: size distribution and aerosol light extinction characteristics. The function that combines these two properties is the specific extinction coefficient. Basically, it is a mass-weighted average of the aerosol mass extinction coefficient.

The inherent error in the program (generally less than about 4 percent) is small when compared to the error in the measurements of the input data. The critical data that control the accuracy of the in-stack opacity prediction are the particle size and mass concentration measurements.

Program Error

The inherent error in the program is defined as the error introduced strictly by the program operation and not by measurement error of the input data. The inherent errors are small and much less than errors in measurement of physical and optical properties of the aerosol emissions. However, the uncertainty in a prediction is a product of both types of errors. These errors may be cancelled or compounded depending on the bias of the data. Assessment of the bias of particle size data on opacity is discussed later.

The lognormal opacity program has very small error, approximately 1 percent. The most significant portion of this error is attributed to roundoff error in the computer. The other causes of error include truncation of lognormal size distribution below 0.01-μm and above 100-μm particle sizes, integration error, and the approximation of the light extinction efficiency factor for particles larger than 7 μm diameter and 0.55 μm light wavelength. The small magnitude of error in this program allows the user to focus on the accuracy of the measurement to determine the quality of the opacity prediction.

This histogram opacity program error is approximately 4 percent, depending on the type of size distribution data. Size distributions close to lognormal distributions or distributions with gradual changes at the ends of the distribution will have less than 4 percent error. Large swings or spikes in the distribution will tend to be lessened by the spline-fitting routine, and errors as great as 15 percent can be generated. Also, the spline interpolation and extrapolation will generate negative values (set equal to zero by the program). This normally occurs at steep decreases in distribution. The mass of particles at these dips is less than 0.01 percent of the total mass. Thus, this interpolation problem creates only a small portion of the total error.

Sensitivity Analysis

The differential method of error analysis for the input parameter error or opacity error shows a one-to-one correspondence for opacity less than 20 percent. For example, a 5-percent error in the mass concentration will cause about a 5-percent error in the in-stack opacity. At low opacities the exponential relationship becomes linear and the opacity error is similar to the input parameter errors.

The input parameters having the largest uncertainty are the particle mass concentration and the specific extinction coefficient.

The mass concentration uncertainty depends mainly on the fluctuation of aerosol emission, stratification in sampling ducts, weighing error of gravimetric technique employed, and gas flow measurements. If proper sampling procedures are followed and the plant emissions are stable, the measurement error should be less than 10 percent.

Determination of the error in the specific extinction coefficient (S_v) is more complex. This parameter is a function of particle size and index of refraction. S_v is most sensitive in those particle sizes corresponding to maximum extinction cross sections or light-scattering efficiencies. The maximum values occur for diameters from 0.2 to 1 μm. If the measured size distribution occurs in this size range and is monodisperse, the measurement error may be multiplied by as much as a factor of three. If most particle sizes are polydisperse and in the size range from 0.2 to 10 μm, the measure-

ment error should not affect opacity prediction by more than 10 percent. The greatest error occurs for the monodisperse particle size distribution. The effect of polydispersity on the specific extinction coefficient for two mass diameters, 0.8 and 1.0, with a refractive index = 1.54-0.01i and $\lambda = 0.55$ μm is:

σ_g	S_v(DG=0.8)	S_v(DG=1.0)
1	7.67	4.68
2	5.66	4.99
4	3.815	3.667
6	3.136	3.062
8	2.77	2.725
10	2.54	2.51

The effect of size distribution on the specific extinction coefficient (S_v) for lognormal distributions can also be seen in Figure 6. This curve was generated from solutions to the Mie equations outlined earlier. These curves are the inverse of the "K" curves originally reported by Ensor (1972) and Ensor and Pilat (1971). S_v is most sensitive to change where the slopes of the curves are the steepest. Clearly, the monodisperse case shows the greatest sensitivity from the 0.1- to 1-μm size range. This curve can be used to determine qualitatively the error in the opacity prediction from particle sizing errors for lognormal or near-lognormal distributions.

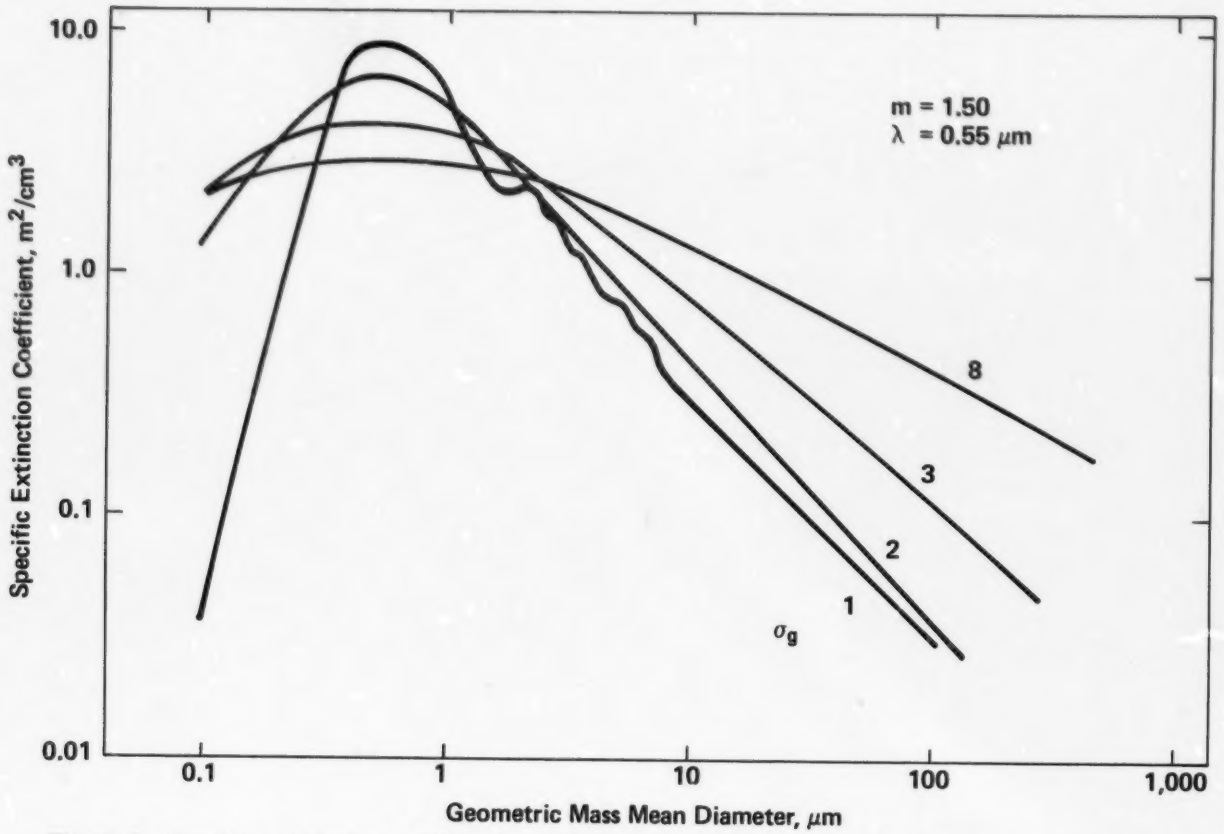

Figure 6. Specific extinction coefficient as a function of lognormal size distribution parameters.

SECTION 4

PROGRAMMER'S GUIDE

This programmer's guide gives details of the program structure for both lognormal and histogram opacity programs. This section can be used either to modify the program or to adapt it for use on other systems. The theory and algorithms were given in Section 3. Some duplication is necessary, but the reader should refer to Section 3 for detailed descriptions of the formulas. This section defines all symbols in the program and program structure or logic. Also, the end of this section is devoted to a systematic approach to debugging the programs. The user should be familiar with the TRSDOS and Disk Reference Manual, 1978, Radio Shack, Ft. Worth, TX 76102.

LOGNORMAL OPACITY PROGRAM

The lognormal opacity program can be divided into four main areas:

1. Menu data input.
2. Subroutine to calculate extinction efficiency and particle size distribution.
3. Romberg integration.
4. Opacity calculation and output results.

Some of these areas are common to the histogram opacity program. Except for changes (such as variable names), these common areas are described only in this part. The listing of the lognormal opacity program is given in Appendix A.

A description of the program logic using block diagrams is shown in Figure 7. This program applies a sample design to facilitate adapting and understanding the program.

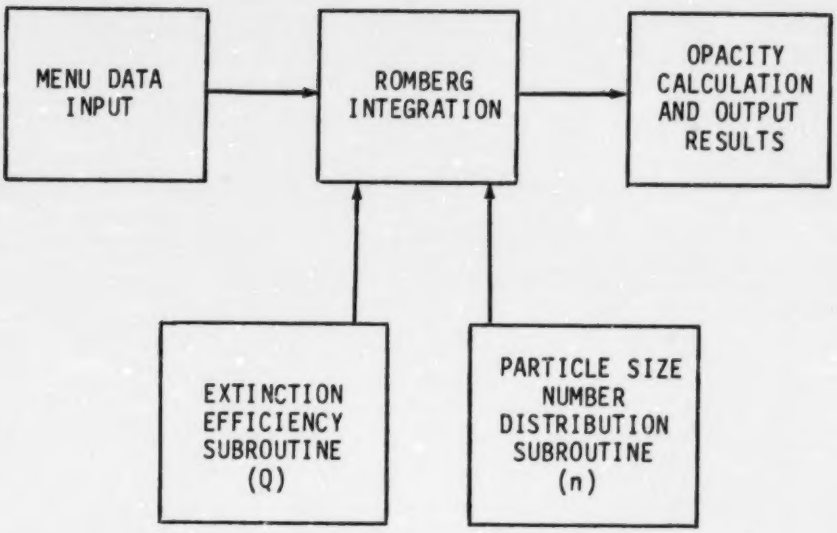
MENU DATA INPUT
ROMBERG INTEGRATION
OPACITY CALCULATION AND OUTPUT RESULTS
EXTINCTION EFFICIENCY SUBROUTINE (Q)
PARTICLE SIZE NUMBER DISTRIBUTION SUBROUTINE (n)

Figure 7. Lognormal opacity program logic.

Lognormal Opacity Program Variable List

Tables 1 through 6 contain all the variables and strings in the lognormal opacity program. This list should help the user avoid duplication of variable names if the program is extended and should facilitate debugging or modification of the program. The variables are listed by order of appearance in each subprogram to help the user find items. Some variables such as T_1, T_2, and T_3 are used more than once because they serve only as temporary storage for intermediate calculations.

Menu Data Input

The data input is accomplished by means of a "menu" in which the user is presented with a list of variables. The user then enters data as indicated by the arrow (→). Before the menu appears on the screen, introductory material is presented, describing program operation and initialization. These features, in the order of the program control, are:

		Line Numbers
1.	Program identification.	10-57
2.	Dimension and description of variables and default values.	100-370
3.	Opacity program HELP routine.	6090-6210
4.	Line printer option	430-510
5.	User comment entry.	530-560
6.	Data input initialization and formatting.	5990-6070

The use of the INKEY$ allows the user to press any key to go quickly and easily through the program preliminaries. When "yes" or "no" questions are indicated (such as the use of the line printer), pressing Y or N is all that is required of the user. Again, strings are used to achieve these quick screen manipulations.

Figure 8 summarizes the menu data input. The menu data input is initiated by calling subroutine 4600. First, the value of IP is set equal to 3 for cursor placement on the CRT. The next subroutine, 4890, prints the data page on the control, screen including all input data descrip-

TABLE 1. INPUT VARIABLES AND VARIABLES USED TO CALCULATE PARTICLE SIZE DISTRIBUTION FOR LOGNORMAL PROGRAM

Symbol	Program variable	Meaning	Default value
n_1	MR	Real part of particle index of refraction	1.5
n_2	MI	Imaginary part of particle index of refraction	0
	(Note:	The refractive index is in the form, MR - MI · i)	
L	L	Wavelength of light (μm)	0.55
M	M	Particle mass concentration (g/m^3)	0.01
ρ	P	Particle density (g/cm^3)	2.4
S	S	Stack diameter (m)	6.9
d_g	DG	Geometric mass mean diameter (μm)	1.0
σ_g	SG	Geometric standard deviation	2.0
n	N	Particle size distribution (number)	--
D_0	DO	Geometric number mean diameter	--
$\ln 0.5 - \frac{d_p}{Do}$	T2	Natural logarithm (0.5 - DP/DO)	--
d_p	DP	Particle diameter	--
$\ln(\sigma_g)$	T3	Natural logarithm of geometric standard deviation	--
-	T6	T2/T3	--
π	PE	Pi (3.141593)	--

Hyphen indicates variable appears only in the computer program.

TABLE 2. INTEGRATION VARIABLES FOR LOGNORMAL PROGRAM

Symbol	Program variable	Meaning
H	H	Integration interval
d_1	D1	Lower integral particle diameter boundary
d_2	D2	Upper integral particle diameter boundary
K%	K%	Superscript in Romberg difference algorithm
k1%	K1%	K% plus 1
-	CT%	Number of terms in integral
-	T1	Particle diameter times number particle size distribution
-	T1	Integral value of light extinction for a given decade
-	T2	Integral value of volume particle size distribution for a given decade
-	T3	Integral value of number particle size distribution for a given decade
-	I1	T1 · light extinction efficiency factor, Q
-	I2	T1 · particle diameter.
W1	W1(10,10)	Romberg difference integral for extinction
W2	W2(10,10)	Romberg difference integral for particle volume
W3	W3(10,10)	Romberg difference integral for number of particles
-	F1	Previous value of I1
-	F2	Previous value of I2
-	F3	Previous value of N
-	S1	Summation of I1
-	S2	Summation of I2
-	S3	Summation of N
-	M%	$2^{(K\%-1)}$
-	L%, LU%, L1%, LV% LM%	These variables are used to identify the terms in the iterative solution
$F_a^{(o)}$	A1	Difference between integral extinction results; i.e., W1(1,LV%) - W1(1,LM%)
-	ER	Integration tolerance

TABLE 3. VARIABLES USED TO CALCULATE EXTINCTION EFFICIENCY

Symbol	Program variable	Meaning
Q	Q	Light extinction efficiency factor
x	XI	Nondimensional particle size parameter; i.e., $\pi \cdot d_p/L$
-	SM	Summation of terms in the Q calculation
-	N1%	Number of terms in Q calculation; i.e., $4 \cdot XI^{1/3} + XI$
$Re[W_n(X)]$	WR(56)	Real part of the complex variable, w_n (XI), used in calculation of Mie coefficients
$Im[W_n(X)]$	WI(56)	Imaginary part of the complex variable, W_n (XI), used in calculation of Mie coefficients
$n_1 \cdot X$	PP	Product of real part of refractive index, MR, and size particle, XI
$n_2 \cdot X$	QQ	Product of imaginary part of refractive index, MI, and size particle, XI
-	TT	Intermediate variable to calculate A_n or a_n
-	SH	$\frac{1}{2} \cdot \left(\frac{TT-1}{TT}\right)$ for TT = EXP(QQ)
-	CH	$\frac{1}{2} \cdot \left(\frac{TT+1}{TT}\right)$ for TT = EXP(QA)
-	T4	SIN(PP)
-	T5	$T4^2 + SH^2$
$Re[A_n(Y)]$	AR(56)	Real part of the complex variable used in calculation of Mie coefficients, A_n
$Im[A_n(Y)]$	AI(56)	Imaginary part of the complex variable used in calculation of Mie coefficients, A_n
-	I%	Iterative variable in calculation of Q
-	I1%	I% - 1
-	I2%	I% - 2
-	PR	Real part of intermediate variable used to calculate real part of A_n, W_n, a_n, or b_n
-	PI	Imaginary part of intermediate variable used to calculate imaginary part of A_n, W_n, a_n, or b_n

TABLE 3 (continued)

Symbol	Program variable	Meaning
-	QI	Imaginary part of intermediate variable used to calculate imaginary part of A_n, a_n, or b_n
-	QR	Real part of intermediate variable used to calculate real part of A_n, a_n, or b_n
$Re[a_n(m,x)]$	ER(56)	Real part of the complex variable, a_n, used to calculate extinction efficiency
$Im[a_n(m,x)]$	EI(56)	Imaginary part of the complex variable, a_n, used to calculate extinction efficiency
-	Y1	Absolute value of a_n or b_n
-	T1	Intermediate imaginary variable used to calculate a_n or b_n
-	TR	Intermediate real variable used to calculate a_n or b_n
$Re[b_n(m,x)]$	FR(56)	Real part of complex variable, b_n, used to calculate extinction efficiency
$Im[b_n(m,x)]$	FI(56)	Imaginary part of complex variable, b_n, used to calculate extinction efficiency
-	UR	Real part of intermediate variable used to calculate b_n
-	UI	Imaginary part of intermediate variable used to calculate b_n

TABLE 4. OUTPUT VARIABLES USED TO COMPUTE OPACITY FOR LOGNORMAL PROGRAM

Symbol	Program variable	Meaning
-	NN%	Number of decades in the integration
-	DI(5)	Values of integral range 0.01, 0.1, 1, 10, 100
-	D1	Lower integral range for a given decade
-	D2	Upper integral range for a given decade
-	V1	Sum of integrals for each decade for extinction
-	V2	Sum of integrals for each decade for volume
-	V3	Sum of integrals for each decade for number
S_v	SP	Specific extinction coefficient (m^2/cm^3)
-	OP	% opacity

TABLE 5. MENU VARIABLES FOR LOGNORMAL PROGRAM

Program variable	Meaning
MX,IP	Variables used to place cursor in correct vertical position
X	ASCII code (in decimal form) of X$ used to obtain an unshifted character from keyboard
DD	This variable is used to increment IP and move cursor
JP	Variable used to control numerical data input
CC	Variable used to place cursor in correct horizontal position
Y	Variable used to obtain numerical input from keyboard

TABLE 6. STRING LISTS FOR LOGNORMAL PROGRAM

Program variable	Meaning
Y$	All-purpose, for keyboard interactions, and to store numerical input data
C$(3)	Stores comments and user descriptions
A$	Used with line printer option
X$	Stores unshifted character from keyboard
P1$	Stores the format and description of the real part of the index of refraction
P2$	Stores the format and description of the imaginary part of the index of refraction
P3$	Stores the format and description of the wavelength
P4$	Stores the format and description of the mass concentration
P5$	Stores the format and description of the particle density
P6$	Stores the format and description of the stack diameter
P7$	Stores the format and description of the mass mean diameter
P8$	Stores the format and description of the geometric standard deviation

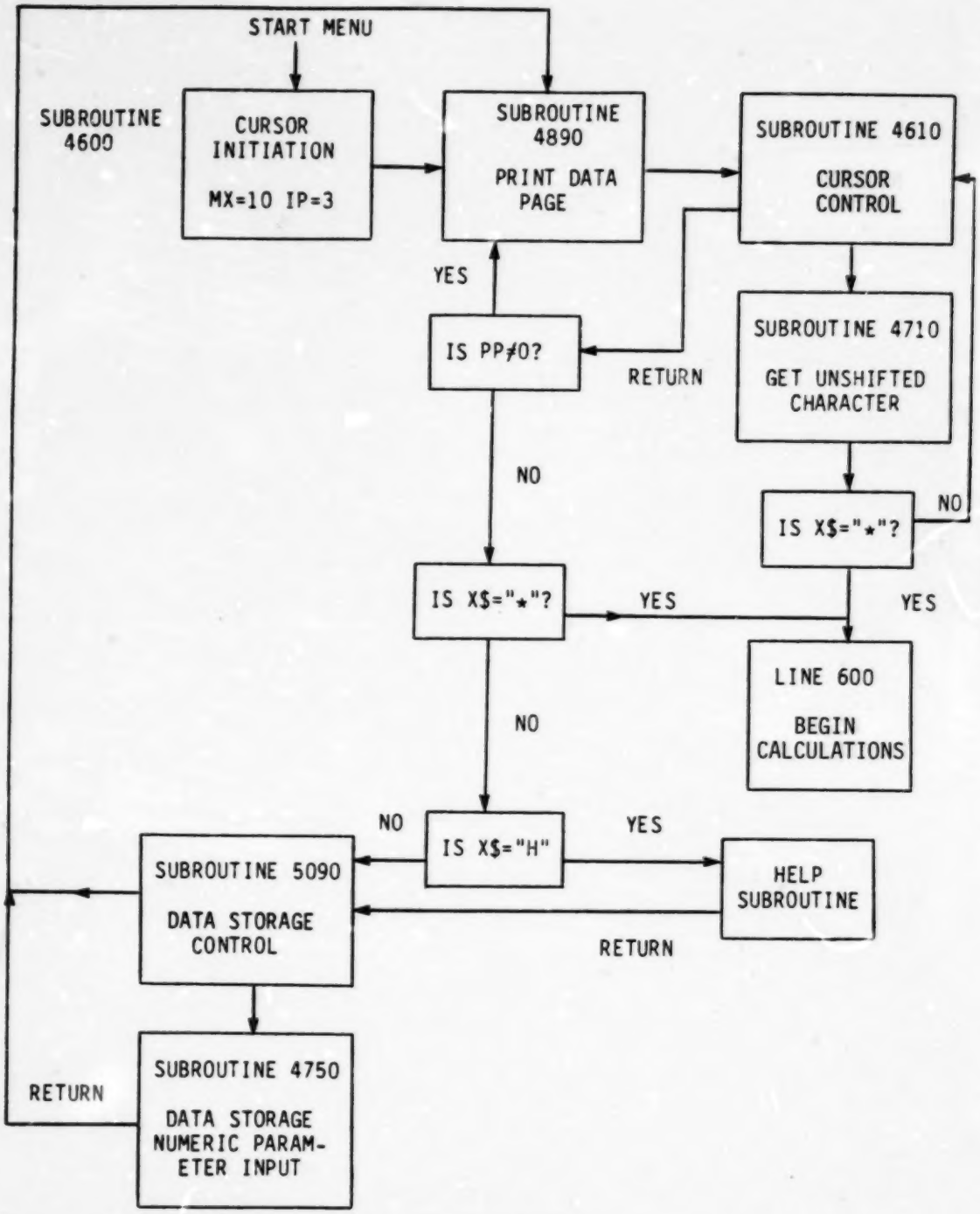

Figure 8. Menu block diagram for lognormal program.

tions, units, and cursor control instructions. The next subroutine, 4610, controls the cursor so that it will move to the next line after each datum is entered.

The first step in subroutine 4610 is to place the cursor (→) at the top of the page by the entry labelled the REAL PART OF INDEX OF REFRACTION. The next step is to call subroutine 4710 to get an unshifted character from the keyboard. If * is pressed, the program will start execution at line 600. If the ASCII value (X) of X$ obtained from keyboard entry is greater than 95 (i.e., lower case characters), 32 is subtracted (to obtain upper case value) from X. X$ is then the character string or CHR$ of this new value of X (CHR$ performs the opposite function of ASC).

The variable DD controls the vertical movement of the cursor. If X equals 27 or 91 (↑), DD equals -1 and the cursor will move up. If the cursor is at the top, the ↑ entry will send the cursor to the bottom line. If X equals 26, 10, or 13, DD equals 1 and the cursor will move down. If the cursor is at the bottom line and ↓ is pressed, the cursor will move to the top line.

If the X$ is equal to H, the HELP subroutine is called to review the program user's instructions.

The next subroutine calls data storage control at line 5090. The variable Y or ASC (Y$) is the numerical input obtained calling subroutine at 4750. The data storage control uses the cursor location, IP, to identify and store the appropriate variable corresponding to the variable description on the screen.

The cycle of menu data input is then completed. The data page is then printed again at line 4890 with the cursor updated to the next lower position.

Extinction Efficiency and Particle Size Distribution Calculations

The light extinction efficiency factor, Q, and the particle size distribution, n, are calculated by using subroutines at lines 1390 and 840, respectively. These subroutines are called by the Romberg integration routine at particle diameters, d_p, during the integrating process.

Light Extinction Efficiency Subroutine--

This subroutine is the most time consuming part of the opacity program. The number of terms in the calculation is a function of the particle size

parameter, XI. This quantity is computed at line 1450. The extinction efficiency for value of XI greater than 40 (7-μm particle diameter at 0.55-μm wavelength) is approximated to the value of 2. This test is performed in line 1420.

The equations used in the calculation of the light extinction efficiency, Q, are identical to the equations cited in Section 3, except that algebraic manipulations are used to reduce the number of calculations and thus reduce computing time. The variable names used in these equations are related to the variables in Section 3 formulations by the list of extinction efficiency variables presented at the beginning of this section. These calculations, in their order of appearance, are:

Lines 1480-1485	Calculation of $W_n(1)$ and $W_n(2)$
Lines 1510-1560	Calculation of $A_0(m,x)$
Lines 1570-1660	Calculation of $W_n(x)$, $A_n(m,x)$
Lines 1690-1750	Calculation of Mie coefficients, $a_n(m,x)$
Lines 1780-1840	Calculation of Mie coefficients, $b_n(m,x)$
Line 1850	Calculation of summation of the Mie coefficients
Line 1870	Calculation of light extinction efficiency factor, Q .

Subroutine to Calculate Number Particle Size Distribution--

This subroutine at lines 840-910 rapidly calculates the particle frequency, n, as a function of particle size for lognormal particle size distributions. The first step is the calculation of the conversion of the geometric mass mean diameter, DG, to the geometric number mean diameter, DO. This conversion is required by the integrals used to calculate the specific extinction coefficient. The remainder of this calculation follows the formulation outlined in Section 3.

Romberg Integration Subprogram

This integration procedure applies the Romberg algorithm to converge on the solution rapidly. Figure 9 describes the subprogram logic. The subprogram occupies lines 920 to 1385.

The first step in the integration is to set the counter k% equal to 0; 2^k is the number of intervals in the integration. The initial mesh size,

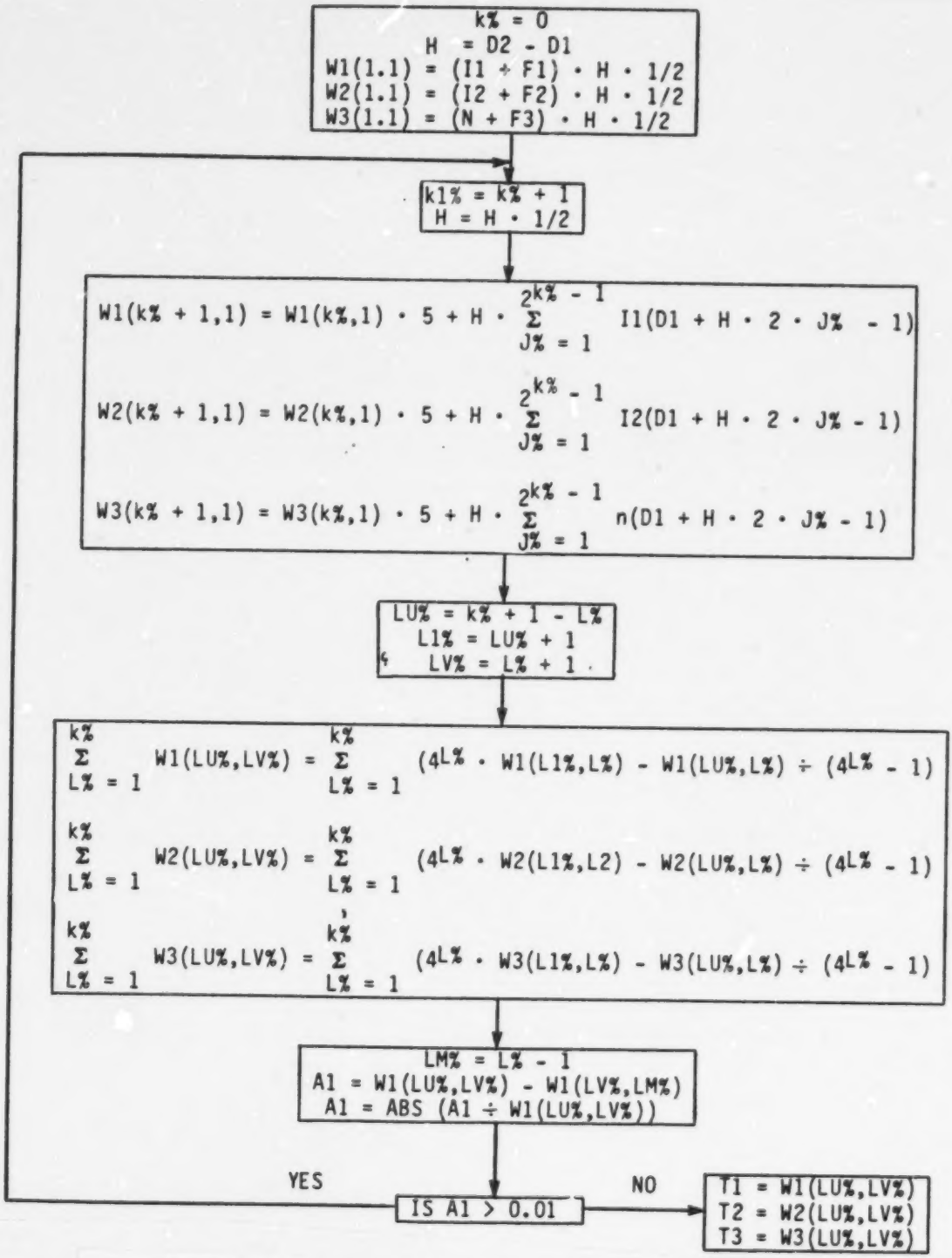
k% = 0
H = D2 - D1
W1(1.1) = (I1 + F1) · H · 1/2
W2(1.1) = (I2 + F2) · H · 1/2
W3(1.1) = (N + F3) · H · 1/2
k1% = k% + 1
H = H · 1/2
W1(k% + 1,1) = W1(k%,1) · 5 + H · Σ I1(D1 + H · 2 · J% - 1)
W2(k% + 1,1) = W2(k%,1) · 5 + H · Σ I2(D1 + H · 2 · J% - 1)
W3(k% + 1,1) = W3(k%,1) · 5 + H · Σ n(D1 + H · 2 · J% - 1)
LU% = k% + 1 - L%
L1% = LU% + 1
LV% = L% + 1
W1(LU%,LV%) = (4^L% · W1(L1%,L%) - W1(LU%,L%) ÷ (4^L% - 1)
W2(LU%,LV%) = (4^L% · W2(L1%,L2) - W2(LU%,L%) ÷ (4^L% - 1)
W3(LU%,LV%) = (4^L% · W3(L1%,L%) - W3(LU%,L%) ÷ (4^L% - 1)
LM% = L% - 1
A1 = W1(LU%,LV%) - W1(LV%,LM%)
A1 = ABS (A1 ÷ W1(LU%,LV%))
YES
IS A1 > 0.01
NO
T1 = W1(LU%,LV%)
T2 = W2(LU%,LV%)
T3 = W3(LU%,LV%)

Figure 9. Subprogram logic diagram describing Romberg algorithm.

H, is upper diameter, D2, less the lower diameter, D1. The first value of the integral is the initial trapezoidal calculation:

$$W1 = f(D2) - f(D1) \cdot H \cdot 1/2 \tag{31}$$

where

W1 = the value of the integral, and

f = the function inside the integral.

The counter k% is then incremented by 1 and the mesh size, H, is halved. This doubles the number of intervals.

The next box in Figure 9 shows the continuation of the trapezoidal rules as a function of the counter, k%. The mesh size, H, is:

$$H = \frac{f(D2) - f(D1)}{2^{k\%}} . \tag{32}$$

The next step defines the variables, LU%, L1, and LV%, in terms of the original counter k% and the new counter L% to simplify identification of the terms in the Romberg difference algorithm. The general equation of this algorithm, shown in the next box in Figure 9, is:

$$W_L(k) = \frac{4^L W_{L-1}^{(k+1)} - W_{L-1}^{(k)}}{4^L - 1} \tag{33}$$

for

$L = 1,2,\ldots$ and $k = 0,1,2,\ldots$.

The value of the extinction integral is tested against the tolerance of 0.01 by computing the value of the integral, W1(LU%, LV%), less the previously calculated value, W1(LU%, LM%), divided by the integral value, and then comparing this quantity to the integral tolerance. If the tolerance is not acceptable, the value of k% is incremented by 1, the mesh size is halved (doubling the number of intervals), and the integral is recalculated.

Opacity Calculations and Output of Results

The integration is performed over four decades from particle diameters of 0.01 to 100 μm. The controlling loop for this integration is found on lines 1910 to 2000. The upper and lower diameters for each integral part

are stored in the dimensional variable, DI(5). The sum of the integral parts, T_1, T_2, and T_3, is stored in the cumulative integrals V1, V2, and V3.

The calculation of the specific extinction coefficient and in-stack opacity is performed on lines 4422 and 4424, respectively. The data are output to the CRT or line printer in lines 4430 to 4500.

The user is asked if another run is desired on lines 4550 and 4560.

HISTOGRAM OPACITY PROGRAM

The histogram program listing is in Appendix B for reference to aid in modification or troubleshooting. The program logic can be divided into eight main areas:

1. Menu data input.
2. Normalization of cumulative particle size distribution.
3. Lognormal transformation of particle size data.
4. Calculation of lognormal fit of particle size data.
5. Subroutine to calculate extinction efficiency.
6. Spline fit of particle size data.
7. Trapezoid integration plus controlling loops.
8. Opacity calculation and output of results.

The program logic is similar to the logic of the lognormal program, except that additional steps are required for particle size data manipulation. Figure 10 shows the basic interactions for the histogram program.

The particle size data are entered using fractional cumulative less than mass vs. particle size. The first manipulation involves transformation of these data into a logarithmic form. A least-squares fit of these data provides the user with an assessment of the lognormal characteristic of the particle size distribution for information purposes only. The logarithmically transformed data are then fit to a natural cubic spline curve for interpolating and extrapolating values of the particle size distribution.

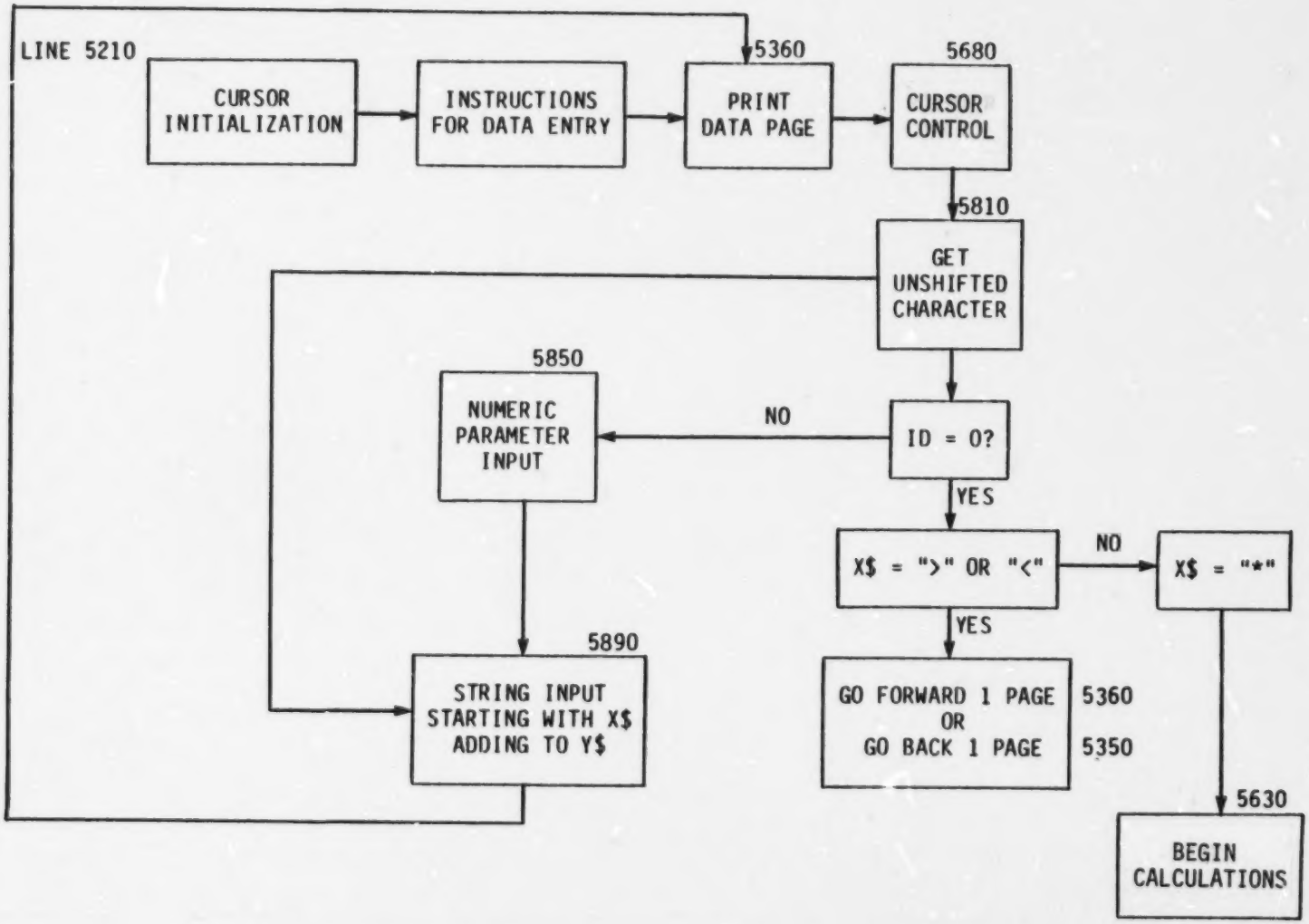

Figure 10. Block diagram showing flow of data in the opacity histogram program.

The normal trapezoid integration calculates extinction for particles in the size range of 0.01- to 100-μm diameters. Similar to the lognormal opacity program, the subroutines to calculate light extinction efficiency and the particle frequency distributions are used to calculate the integrands.

Histogram Opacity Program Variable List

Tables 7 through 14 contain all the variables and strings in the histogram opacity program. This list should help the user avoid duplication of variable names if the program is extended and should facilitate debugging or modification of the program. Most of the variable names are identical to those in the lognormal opacity program.

The light extinction subroutine and variable list for the histogram program is identical to the one used in the lognormal opacity program. The user should consult the lognormal opacity list (Table 3) for questions relating to this subroutine.

Menu Data Input

The introductory program material (including program ID, dimension and variable description, HELP subroutine, line printer option, user comment entry, and data input initialization and formatting) is also very similar to that of the lognormal opacity program.

The menu data input for the first data page is nearly identical to that for the lognormal opacity program. The user should refer to that discussion for this information. The following data pages are used to enter particle size distribution data. Figure 11 summarizes particle size distribution data entry. The flow of information is very similar to the other menu routine except that numeric data storage in this case involves string manipulations at line 5890.

The menu for particle size data is initiated at line 5210 where cursor parameters JS, MX, JL, and IL are set. The first information appearing on the screen is the user instruction on entering particle size and cumulative mass fraction data. The next page appearing will be the page used for the particle size distribution data entry. The subroutine at 5680 then controls the cursor (pointer). The steps in this routine basically cause the cursor

TABLE 7. INPUT VARIABLES FOR HISTOGRAM PROGRAM

Symbol	Program variable	Meaning
n_1	MR	Real part of particle index of refraction
n_2	MI	Imaginary part of particle index of refraction
	(Note: The refractive index is in the form MR - MI · i)	
λ	L	Wavelength of light (μm)
m	M	Particle mass concentration (g/m^2)
ρ	P	Particle density (g/cm^3)
L	S	Stack diameter (m)
n	N%	Number of particle diameters input
-	D(27)	Particle diameters (μm)
-	F(27)	Cumulative less than mass fractions

TABLE 8. VARIABLES USED IN LOGNORMAL TRANSFORMATION

Symbol	Program variable	Meaning
C_0, C_1, C_2 D_1, D_2, D_3	C0, C1, C2 D1, D2, D3	Constants used in polynomial expression to invert normally transformed data
Y	X(27)	Logarithm of particle diameters
-	LT	Conversion factor to change natural logarithm to logarithm Base 10
-	PL%	Flag for cumulative mass fraction either greater or less than 1/2
F	CU	Value of cumulative mass fraction
-	T	Square root of [-2 · log (CU)]
YY	Y(27)	Logarithmic transformation of cumulative mass fraction data
-	TX, TY	Variables used to store X(I%) and Y(I%) to reverse the order of the data

TABLE 9. VARIABLES FOR LEAST-SQUARES FIT

Program variable	Meaning
XN%	Counter variable used to define number of data points
SX	Sum of X(I%) on lognormally transformed particle diameter
SY	Sum of Y(I%) on lognormally transformed cumulative mass
XY	Sum of the product of X(I%) and Y(I%)
XX	Sum of the square of X(I%)
YY	Sum of the square of Y(I%)
B	Function used to calculate lognormal parameters
A	Function used to calculate lognormal parameters
R	Correlation coefficient
DG	Geometric mass mean diameter (μm)
SG	Geometric standard deviation

TABLE 10. SPLINE FIT VARIABLES

Program variable	Meaning
OM	Relaxation parameter
H(27)	ΔX_i, also difference between successive dependent data points
DL(27)	$\Delta Y_i / \Delta X_i$, slope of line between successive data points
H2(27)	ΔH_i, second differences of X values
BL(27)	$1/2 \cdot H/\Delta H$
DQ(27)	$\Delta DL/\Delta H$
S2(27)	$2 \cdot DQ$, second derivative of spline curve
C(27)	$3 \cdot DQ$, spline parameter C is the coefficient to X^2 term
W	Incremental second derivative solution to spline curve fit
ET	Tolerance for overrelaxation technique
S3(27)	$\Delta S2/\Delta X$, also third derivative of spline curve

TABLE 11. VARIABLES FOR INTERPOLATING PARTICLE SIZE FREQUENCY DISTRIBUTION

Program variable	Meaning
XI	Particle diameter
XX	Logarithm of particle diameter
S1	First derivative of spline curve fit through the data
YY	Logarithm of cumulative mass function corresponding to particle diameter, XX
H1	XX - X(I%)
H2	XX - X(I% + 1)
PR	H1 · H2
Y2	S2 + (H1 · S3)
DQ	Intermediate result used to calculate the transformed cumulative mass function
Y1	First derivative of the transformed cumulative function
DG	Proportional to volume particle size distribution, also first derivative of cumulative mass curve
XD	Proportional to frequency (number) particle size distribution

TABLE 12. INTEGRATION, CONTROLLING LOOP, AND OUTPUT VARIABLES FOR HISTOGRAM PROGRAM

Program variable	Meaning
V1	Proportional to total particle light extinction integral
V2	Proportional to total particle volume integral
V3	Proportional to total particle frequency (number) integral
D1	Lower bound to integral
D2	Upper bound to integral
FR%	Flag in the trapezoid integration used to calculate integral increment
T1	Proportional to particle light extinction integral for particle size interval, D2 - D1
T2	Proportional to particle volume integral for particle size interval, D2 - D1
T3	Proportional to particle number integral for particle size interval, D2 - D1
Z1	XD · DP^2, used to calculate part of the integrand
XD	Frequency (number) particle size distribution
(Note:	This variable (XD) has the different symbol, N, in lognormal program.)
I1	Extinction integrand
I2	Volume integrand
DT	Logarithmic particle diameter interval size
DX	Stores particle diameter, DP, to compute interval size
L1	Stores extinction integrand, I1, to complete trapezoid computation
L2	Stores volume integrand, I2, to complete trapezoid computation

TABLE 12 (continued)

Program variable	Meaning
XL	Stores number integrand, XD, to complete trapezoid computation
EX(27)	Extinction percentage per particle size interval
VO(27)	Volume percentage per particle size interval
XU(27)	Number percentage per particle size interval
SP	Specific extinction coefficient (m^2/cm^3)
OP	Opacity (%)

TABLE 13. MENU VARIABLES FOR HISTOGRAM PROGRAM

Program variable	Meaning
MX, IP, IL	Places cursor in correct vertical position
X	ASCII code (decimal form) of X$, obtains an unshifted character from keyboard
DD	Increments IP and moves cursor
JP	Controls numerical data input
CC	Places cursor in correct horizontal position
Y	Obtains numerical input from keyboard
PP	Flags the program for data entry or continues to calculations or HELP subroutine
J, JS, JL, NJ	Prints size distribution entry page
IC	Places cursor in either particle diameter column or cumulative mass fraction column
ID	Moves cursor to the right and down the particle size distribution entry page

TABLE 14. STRING LIST FOR HISTOGRAM PROGRAM

Program variable	Meaning
Y$	All-purpose, for keyboard interactions, and to store numerical input data
R$(3)	Stores comments and user descriptions
A$	Used with line printer option
X$	Stores unshifted character from keyboard
P1$	Stores the format and description of the real part of index of refraction
P2$	Stores the format and description of the imaginary part of index of refraction
P3$	Stores the format and description of the wavelength
P4$	Stores the format and description of the mass concentration
P5$	Stores the format and description of the particle density
P6$	Stores the format and description of the stack diameter

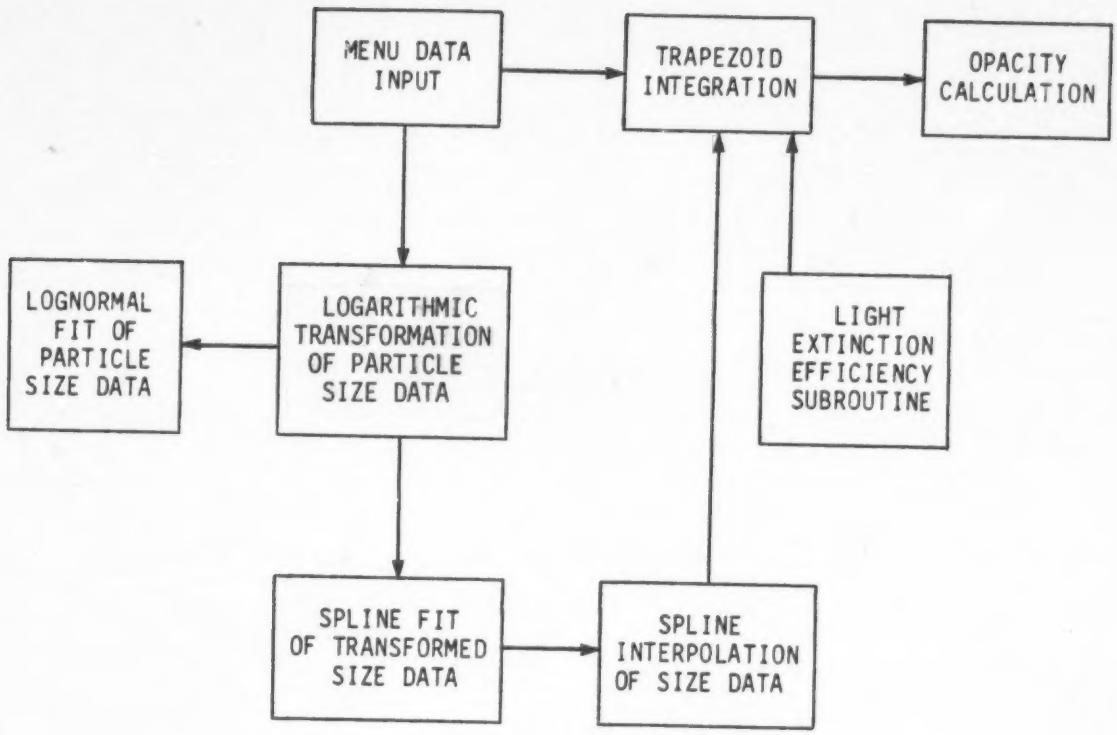
MENU DATA INPUT
TRAPEZOID INTEGRATION
OPACITY CALCULATION
LOGNORMAL FIT OF PARTICLE SIZE DATA
LOGARITHMIC TRANSFORMATION OF PARTICLE SIZE DATA
LIGHT EXTINCTION EFFICIENCY SUBROUTINE
SPLINE FIT OF TRANSFORMED SIZE DATA
SPLINE INTERPOLATION OF SIZE DATA

Figure 11. Menu block diagram for histogram opacity program.

to be moved by the ↑, ↓, →, or ←. The cursor is placed initially at the first particle diameter at the top left corner.

If * is pressed, program calculations will begin (line 5630). If a previous data entry page (<) or following page (>) is desired, the program is returned to line 5350 or 5360, depending on the user key entry.

If a numeric parameter is input, the program logic goes to the subroutine at line 5850. String manipulations then occur at line 5890 with Y$ storing the numeric information. The cursor parameters are adjusted so that the cursor will move to the right side if it started on the left, or down and to the left if it started on the right. The subroutine at 5810 that handles the unshifted character can also be called if the user detects an error in previously entered numerical data.

The Light Extinction Efficiency Calculation

This calculation is identical to the one in the lognormal opacity program. The user should refer to that discussion for a detailed description.

Integration and Controlling Loop Calculations

The general flow of data is shown in Figure 10. The actual program statements can be categorized into three parts:

1. Controlling loop that defines the upper and lower bounds of each subintegral (lines 1309-1321).

2. Cumulation of integral parts and intermediate output (lines 3002-3018).

3. Calculation of integrands (lines 850-1040).

The controlling loop begins at line 1309 by setting the initial value of the three integrals, V1, V2, and V3, equal to zero. First the lower and upper bounds of the first subintegral are defined to be 0.01 and D(1), respectively. Then the subroutine at line 3004 is called to output the intermediate result, T1, T2, and T3, stored in the total integrals, V1, V2, and V3.

After this initial subintegral has been calculated, the controlling loop sets the lower bound of the next subintegral to D(1) and the upper

bound becomes D(2). This process is repeated until all the integrals have been calculated for each interval in the particle size data. Finally, the lower bound of the final integral is set equal to D(N%) and the upper bound is 100 μm.

The integrals are calculated at line 850 by a trapezoid integration routine. Initially all the integral values are set equal to zero. This integration calls two subroutines to obtain the light extinction efficiency, Q (line 1390), and the particle frequency (number) distribution, XD (line 1338). The number of intervals is determined by the input size distribution data. The integration contains 10 subintervals for each interval in the particle size data. The trapezoid integration simply sums two consecutive functional values and multiplies this sum by 0.5 of the interval size, $\Delta \log D_p$.

Particle Size Distribution Data Manipulation

The particle size distribution data are entered in the form of cumulative mass fractions vs. particle diameters and are transformed into a particle number distribution for computing the integrands. The data undergo a logarithmic transformation and are fitted to a natural cubic spline curve. This curve is then used to interpolate and extrapolate values of the number distribution for particle diameters involved in the integration.

The lognormal transformation is accomplished by the subroutine at line 3280. The lognormal transformation of the particle diameter occurs at line 3371, while the cumulative mass data are transformed (using the inverse normal approximation from Section 3) at line 3420. The data are transposed and sorted so that the X array is in ascending order in lines 3460-3580.

A least-squares fit of the transformed data giving the best lognormal fit is calculated by the subroutine at lines 1070-1230. This procedure is solely for the user's information; it does not enter into any further calculations.

The spline-fitting subroutine at lines 3600-3900 is the BASIC version of a routine given by Lawless (1981). The first differences are computed on lines 3650-3670, second differences on lines 3690-3750, successive over-relaxation solutions on lines 3790-3850, and third differences on lines

3870-3890. The spline parameters computed in this subroutine are saved in arrays and are used for interpolating and extrapolating particle diameters called out by the integration. The subroutine that accomplishes this task occurs at lines 1338-1364.

The spline fit interpolation begins at line 1338 by lognormally transferring the incoming particle diameter. If this value, XX, is equal to X($), then the program transfers to line 1355. The values of the spline derivative at X($) are then used to calculate the number distribution at X(1). If XX is equal to X(N%), the program transfers to line 1353. Values of the particle diameter outside the measured range involve a linear extrapolation at line 1345 for particle diameters smaller than X(%) and at line 1348 for particle diameters greater than X(N%). The interpolating values for particle diameters between X(1) and X(N%) are generated in lines 1353-1364.

OPACITY PROGRAM DEBUGGING PROCEDURE

The procedure for debugging the opacity programs is really not very different from that used for any other computer program. However, certain steps are worth mentioning to facilitate debugging these programs.

The programs should be run first using the BASIC Interpreter so that the user can have an interactive dialogue with the program. This dialogue will allow easy identification of the problem, if not its solution. This program can be stopped at any point by pressing BREAK; it can be restarted by typing CONT and pressing ENTER. This allows the user to stop the program during intermediate calculations so that intermediate variables can be printed either on the CRT or line printer. Also, if the program crashes when dividing by zero, the line number of the error will be shown on the screen.

Another feature of the TRS-80 that is useful in debugging is the trace mode. This allows the user to follow the progression of the program so that the correct switches and routings through the program are made. However, the trace mode should be used only immediately before pressing * to start calculations. Otherwise the user will not be able to follow the directions of the menu data input because the internal loops in the menu will cover the entire screen before the user can react. The trace

mode is initiated by typing TRON and pressing ENTER. Then type RUN and press ENTER to start the program. If the user wants the trace mode inactivated, type TROFF and press ENTER.

The debugging procedure consists of three general steps:

1. Run the sample case using the BASIC Interpreter.

2. Check the subroutines used to calculate (a) the light extinction efficiency factor and (b) the particle number size distribution.

3. Use the trace mode to follow the program progression to ensure correct information flow.

Step 1 simply runs the sample case built into the programs. If the same results are obtained, the debugging procedures are unnecessary. Be sure that the line printer is ready for use if that option is chosen, otherwise nothing will happen. The program should be run on the BASIC Interpreter so that any syntax errors caused by typographical errors can be found and easily corrected. The intermediate output values of the integrals should be compared on the histogram opacity program. If these intermediate values agree, the user might then want to compile the program to obtain the final result quickly. Also, if the lognormal opacity program seems to be running without problems, then it can be compiled for faster operation.

If final or intermediate results do not agree with the sample, Step 2 checks the subroutine that calculates extinction efficiency, Q, and the number size distribution (N for lognormal program, XD for the histogram program). This can be done by:

1. Entering the following to get Q manually in BASIC:

```
>MR = 1.525
>MI = 0.0682
>PE = 3.141593
>L = 0.55
>DP = L/PE
>GOSUB 1390 (for Q)
>Print Q
0.419877
```

2. Running the sample program to get the number particle size distribution.

For the histogram opacity program,

when DP = 0.01, N = 6.65261E-04; and
DP = 0.2, N = 21.3348.

For the lognormal opacity program,

when DP = 0.01, N = 1.72213E-03.

If these same results are not obtained, stop the program by pressing BREAK, and print out intermediate results. Another approach is to compare a list of these subroutines, line by line, with the list in Appendix B.

If these subroutines are working properly and the results still do not agree, the user might try the trace mode (Step 3, above) to ensure that transfer from statement to statement is correct. These debugging procedures are not foolproof; they are intended only to guide the user. Careful entry of the program is the best prevention of debugging headaches.

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APPENDIX A

PROGRAM NO. 1: LOGNORMAL OPACITY PROGRAM LISTING

```
10 REM — LOGNORMAL OPACITY PROGRAM — VERSION 1.0
20 REM DELETE STATEMENT  30  TO COMPILE
25 REM PROGRAM ASSEMBLED BY S. COHEN, ATMOSPHERIC RESEARCH GROUP 11/18/80
26 REM PROJECT OFFICER-L.E.SPARKS; ENVIRONMENTAL PROTECTION AGENCY GRANT #R806718010
30 CLEAR 100
40 CLS:PRINTSTRING$(63,"="):PRINT"OPACITY PREDICTION PROGRAM"
50 PRINT STRING$(63,"=")
51 PRINT "THIS PROGRAM WAS DEVELOPED BY "
52 PRINT "S. COHEN (METEOROLOGY RESEARCH INC.)"
53 PRINT "D. ENSOR (RESEARCH TRIANGLE INSTITUTE)"
54 PRINT "L. SPARKS( ENVIRONMENTAL PROTECTION AGENCY)"
55 PRINT "EPA PROJECT OFFICER - L. SPARKS  - GRANT #R806718010"
56 PRINT " PRESS ANY KEY ONLY ONCE.  A PAUSE MAY BE NOTICED WHILE DEFAULT   VALUES  ARE BEING ENTERED."
57 Y$ = INKEY$: IF Y$ = "" THEN 57
100 DIM R$(3)
104 DIM MR(56),MI(56),AR(56),AI(56),ER(56),EI(56),FR(56),FI(56)
106 DIM DI(5),W1(10,10),W2(10,10),W3(10,10)
110 REM  DEFINE VARIABLES AND ARRAYS
120 DEFINT N
130 REM
160 REM MR!    REAL PART OF THE INDEX OF REFRACTION
170 REM  MI!     IMAG PART OF INDEX OF REFRACTION
210 REM  DP!     PARTICLE DIAMTER (VAR. OF INTEG.)
220 REM  FOLLOWING ARE DEFAULT VALUES
230 DI!(1)=.01:DI!(2)=.1:DI!(3)=1.:DI!(4)=10.:DI!(5)=100.
240 MR! = 1.5
250 MI! = 0.0
260 L! = .55
270 SG! = 2.0
280 DG! = 1.0
290 M! = 0.01
300 P! = 2.4
310 S! = 6.9
315 ER! = 0.01
317 REM ER! IS THE ROMBERG INTEGRATION TOLERANCE
320 REM  L!     'WAVELENGTH OF LIGHT (MICRONS)
330 REM  M!     'MASS CONCENTRATION (GMS / CUBIC METER)
340 REM  P!     'PARTICLE DENSITY (GMS/ CC)
350 REM  S!     'STACK DIAMETER (METERS)
360 REM SG! GEOMETRIC STANDARD DEVIATION
370 REM DG! GEOMETRIC MASS MEAN DIAMETER
380 PE!=3.141593
400 LT=LOG(10.0)
410 REM
420 GOSUB 6080
430 CLS:PRINT STRING$(64,"=")
440 PRINT "DO YOU WANT LINE PRINTER OUTPUT?TYPE Y OR N."
450 PRINT :PRINT STRING$(64,"=")
460 Y$=INKEY$:IFY$="" THEN 460 ELSE IF Y$="Y" THEN A$="YES" ELSE IF Y$="N" THEN A$="NO" ELSE PRINT "ANSWER Y OR N":GOTO 460
470 IF A$="YES" THEN PP%=99:GOTO 510
480 IF A$ = "NO"  THEN PP% = 0 : GOTO 510
490 PRINT "CANNOT RECOGNIZE INPUT - TRY AGAIN"
500 GOTO 440
510 REM
520 IF PP% = 0 THEN 570
530 CLS:PRINT STRING$(63,"="):PRINT"YOU MAY ENTER UP TO THREE LINES OF COMMENTS"
540 PRINT"ENTER COMMENTS AND PRESS ENTER AFTER EACH LINE"
550 PRINT STRING$(63,"=")
560 FOR I = 1 TO 3: LINE INPUT R$(I): IF PP%<>0 THEN LPRINT   R$(I): NEXT I
570 GOSUB 5990
580 GOSUB 4600
590 REM
600 IF PP% <> 0 THEN LPRINT"STACK OPACITY CALCULATION"
610 IF PP%<>0 THEN LPRINT"INDEX OF REFRACTION=",MR,"-",MI,"xI"
```

```
620 IF PP% <> 0 THEN LPRINT "WAVELENGTH =", L!
630 IF PP% <> 0 THEN LPRINT "MASS CONCENTRATION =", M!
640 IF PP% <> 0 THEN LPRINT "PARTICLE DENSITY =", P!
650 IF PP% <> 0 THEN LPRINT "STACK DIAMETER =", S!
660 IF PP% <> 0 THEN LPRINT "GEOMETRIC STD DEV = ", SG!
670 IF PP% <> 0 THEN LPRINT "MASS MEAN DIAMETER= ", DG!
680 CLS
835 IF SG < 1.3 THEN DP = DG: PRINT"THE PROGRAM IS COMPUTING THE MONODISPERSE CASE FOR DG =",DG: GOSUB 1390: SP=1.5 * Q / DP: GOTO
4424
837 GOTO 1985
840 REM  SUBROUTINE TO CALCULATE N!
850 DO!=EXP(LOG(0.5*DG!) - 3.0*(LOG(SG!))^2)
860 T2! = LOG (0.5 * DP! / DO!)
870 T3! = LOG(SG!)
880 T6 = T2 / T3
890 N! = EXP(-.5 * T6 * T6) / (SQR(2.0 * PI) * T3 * DP)
895 IF N! = 0.0 THEN N! = 1.0E-25
910 RETURN
920 REM ROMBERG INTEGRATION SUBPROGRAM
930 H!=.02!-.01!
940 KZ=0:K1Z=0:CTZ=0
950 DP!=.01!
960 GOSUB 840
970 GOSUB 1390
980 T1!=DP!*DP!*N!*.5:I1!=T1!*Q!:I2!=T1!*DP!
990 CTZ=CTZ+1
1000 F1!=I1!: F2!=I2!: F3!=N!
1010 DP!=.02!
1020 GOSUB 840
1030 GOSUB 1390
1040 T1!=DP!*DP!*N!*.5:I1!=T1!*Q!:I2!=T1!*DP!
1050 CTZ=CTZ+1
1060 W1!(1,1)=((I1!+F1!)*H!)*.5
1070 W2!(1,1)=((I2!+F2!)*H!)*.5
1080 W3!(1,1)=((N!+F3!)*H!)*.5
1090 KZ=KZ+1
1100 H!=H!*.5
1110 S1!=0.0: S2!=0.0: S3!=0.0
1120 MZ=2^(KZ-1)
1130 FOR JZ=1 TO MZ STEP 1
1140      J1!=2*JZ-1
1150      DP!=.01!+H!*J1!
1160 GOSUB 840
1170 GOSUB 1390
1180      T1!=DP!*DP!*N!*.5:I1!=T1!*Q!:I2!=T1!*DP!
1190      CTZ=CTZ+1
1200      S1!=S1!+I1!
1210      S2!=S2!+I2!
1220      S3!=S3!+N!
1230 NEXT JZ
1240 K1Z=KZ+1
1250 W1!(K1Z,1)=W1!(KZ,1)*.5+H!*S1!
1260 W2!(K1Z,1)=W2!(KZ,1)*.5+H!*S2!
1270 W3!(K1Z,1)=W3!(KZ,1)*.5+H!*S3!
1280 FOR LZ=1 TO KZ
1290      LUZ=KZ+1-LZ: L1Z=LUZ+1: LVZ=LZ+1
1300      W1!(LUZ,LVZ)=(4.^L1Z*W1!(L1Z,LZ)-W1!(LUZ,LZ))/(4.^LZ-1)
1307 REM
1310      W2!(LUZ,LVZ)=(4.^L1Z*W2!(L1Z,LZ)-W2!(LUZ,LZ))/(4.^LZ-1)
1320      W3!(LUZ,LVZ)=(4.^L1Z*W3!(L1Z,LZ)-W3!(LUZ,LZ))/(4.^LZ-1)
1330 NEXT LZ
1340 LVZ=LZ-1:A1!=W1!(LUZ,LVZ)-W1!(LUZ,LMZ)
1350 A1!=ABS(A1!/W1!(LUZ,LVZ))
1360 IF L1Z>=10 THEN PRINT "ROMBERG PROBLEM"
1370 IF A1!>ER! THEN GOTO 1090
1380 T1!=W1!(1,LVZ): T2! = W2!(1,LVZ): T3! = W3!(1,LVZ)
1385 RETURN
```

```
1390 REM SUBROUTINE TO CALCULATE THE EXACT EXTINCTION EFFICIENCY, Q , USING THE MIE EQUATIONS
1400 REM
1405 IF L! = 0.0 THEN PRINT"WAVELENGTH MUST HAVE POSITIVE VALUE SUCH AS .55;                    PRESS ANY KEY TO CONTINUE"
1407 IF L! =0.0 THEN Y$ = INKEY$: IF Y$ ="" THEN 1407 ELSE 570
1410 XI! = PE! * DP! / L!
1420 IF XI > 40. THEN Q = 2.0: RETURN
1425 IF N!<1E-20 AND N!<> 0 THEN Q! = .001: RETURN
1430 REM USE A VALUE OF 2.0 FOR Q FOR LARGE XI
1440 SN! = 0.0
1450 N1Z = 4.0 * XI!.333 + XI
1460  IF N1Z < 3 THEN N1Z = 3
1470  N1Z = N1Z + 2: 'INCLUDE 0 AND -1 SUBSCRIPTS
1480 MR!(1) = COS (XI): MI!(1) = - SIN(XI)
1485 MR!(2) = SIN (XI): MI!(2) = COS(XI)
1490 REM CALCULATE THE  A(N)
1500 PP! = MR * XI: QQ! = MI * XI
1510 REM SINH(Q) AND COSH(Q)
1520 TT! = EXP(QQ!)
1530 SH! = (TT - 1.0 / TT) * .5
1540 CH! = (TT + 1.0 / TT) * .5
1550 T4! = SIN (PP): T5! = T4 * T4 + SH * SH
1560 AR!(2) = T4! * COS (PP) / T5:  AI!(2) = SH * CH / T5
1570     FOR IZ = 3 TO N1Z
1580       I1Z = IZ - 1:  IZZ = IZ - 2
1590       PR! = (2 * IZZ - 1) / XI
1600       MR(IZ) = PR * MR(I1Z) - MR(IZZ)
1610       MI(IZ) = PR * MI(I1Z) - MI(IZZ)
1620       PR = IZZ / XI: TT = MR * MR + MI * MI
1630       QI = (PR * MI) / TT: QR = (PR * MR) /TT
1640       PR = QR - AR(I1Z):   PI = QI - AI(I1Z)
1650       TT = PR * PR + PI * PI
1660      AR(IZ) = PR / TT - QR: AI(IZ) = -PI / TT - QI
1670       Y1 = ABS (ER(I1Z)) + ABS (EI(I1Z))
1680         IF IZ > 3 AND Y1 < 1.0 E-20 THEN ER(IZ) = 0.0:    EI(IZ) = 0.0 : GOTO 1760
1690            TT = MR * MR + MI * MI
1700            TI = (AI(IZ) * MR + AR(IZ) * MI) /TT
1710            TR = (AR(IZ) * MR - AI(IZ) * MI) / TT +IZZ / XI
1720            PR = TR * MR(IZ) - MR(I1Z): PI = TI *MR(IZ)
1730            QR = TR * MR(IZ) - TI * MI(IZ) - MR(I1Z): QI = TR * MI(IZ) + TI * MR(IZ) - MI(I1Z)
1740            TT = QR * QR + QI * QI
1750            EI(IZ) = (PI * QR - PR * QI) / TT: ER(IZ) = (PR* QR + PI * QI)/ TT
1760       Y1 = ABS (FR!(I1Z)) + ABS ( FI!(I1Z))
1770       IF IZ > 3  AND Y1 < 1.0 E -20 THEN FR(IZ) = 0.0: FI(IZ) = 0.0 :GOTO 1850
1780            TI = MR * AI(IZ) - MI * AR(IZ)
1790            TR = MR * AR(IZ) + MI * AI(IZ) + IZZ / XI
1800            UR = TR * MR(IZ) - MR(I1Z): UI = TI * MR(IZ)
1810            PI = TR * MI(IZ) + TI * MR(IZ) - MI(I1Z)
1820            QR = TR * MR(IZ) - TI * MI(IZ) - MR(I1Z)
1830            TT = QR * QR + PI * PI
1840            FR(IZ) = (UR * QR + UI * PI) / TT: FI(IZ) =          (UI * QR - UR * PI) / TT
1850       SN = SN + (2 * IZZ + 1) * (ER(IZ) + FR(IZ))
1860       NEXT IZ
1870      Q = 2.0 * SN / (XI * XI)
1880  PRINT "DIAM = ",DP,"Q = ",Q
1890 PRINT "N(DP) =",N!
1900 RETURN
1905 FLI =  0
1910 V1! = 0.0: V2! = 0.0 : V3! = 0.0
1920 FOR NWZ = 1 TO 4
1930      N1Z = NWZ + 1
1940      D1! = DI(NWZ): D2! = DI(N1Z)
1950      PRINT NWZ "LOWER - UPPER DIAM",D1!,D2!
1960     GOSUB 920: ' CALCULATE INTEGRANDS
1970      V1 = V1 + T1: V2 = V2 + T2: V3 = V3 + T3
1980      PRINT "EXTINCTION","VOLUME","NUMBER","NO. TERMS"
```

```
1990     PRINT T1!,T2!,T3!,CT%
2000     NEXT MM%
4420 REM PRINT "INTEGRALS=",V1,V2,V3
4422 SP = 1.5 * V1/V2
4424 OP = 100. * (1. - EXP(-SP * M * S / P))
4430 PRINT""
4440 PRINT "SPECIFIC EXTINCTION COEFFICIENT=",SP
4450 PRINT"MASS CONCENTRATION=",M
4460 PRINT"PARTICLE DENSITY=",P
4470 PRINT "STACK DIAMETER=",S
4480 PRINT "OPACITY(%)=",OP
4490 IF PP% <> 0 THEN LPRINT "SPECIFIC EXTINCTION COEFFICIENT  (M2/CM3) = ", SP
4500 IF PP% <> 0 THEN LPRINT " OPACITY(%) =", OP
4550 PRINT "DO YOU WANT TO RUN ANOTHER CASE? Y OR N"
4560 Y$=INKEY$: IF Y$="" THEN 4560 ELSE IF Y$ ="N" THEN END    ELSE IF Y$="Y" THEN 570 ELSE PRINT "ANSWER Y OR N": GOTO 4560
4600 MX = 10:IP = 3: GOSUB 4890
4610 REM *** POINTER CONTROL FOR MENUES ***
4620 PRINT @IP%64,CHR$(94);
4630 GOSUB 4710
4640 PRINT @IP%64," ";
4650 DD=0
4660 IF X=27 OR X=91 THEN DD=-1
4670 IF X=26 OR X=10 OR X=13 THEN DD=+1
4680 IP=IP+DD : IF IP <1 THEN IP=MX
4690 IF IP>MX THEN IP=3
4700 RETURN
4710 REM *** GET AN UNSHIFTED CHARACTER FROM KEYBOARD ***
4720 X$=INKEY$ : IF X$="" THEN 4720 ELSE X=ASC(X$)
4725 IF X$="x" THEN 600
4730 IF X>95 THEN X=X-32 : X$=CHR$(X)
4740 RETURN
4750 REM *** NUMERIC PARAMETER INPUT USING SUBR @ 1900
4760 PRINT  @IP * 64 + CC, STRING$(9," ");
4770 GOSUB 4790 : Y=VAL(Y$)
4780 RETURN
4790 REM *** STRING INPUT, ADDING TO Y$ STARTING WITH X$ ***
4800 CC=CC+1
4810 Y$=X$
4820 PRINT @IP%64+CC,Y$;CHR$(95);" ";
4830 GOSUB 4710
4840   IF X=13 THEN CC=CC-1 : RETURN
4850   IF X=8 THEN IF LEN(Y$)>0 THEN Y$=LEFT$(Y$,LEN(Y$)-1)
4860   IF X=24 THEN Y$=""
4870   IF X>31 THEN Y$=Y$+X$
4880 GOTO 4820
4890 CLS
4895 MX = 10: IF IP < 3 THEN IP = 10
4900 PRINT STRING$(63,"=")
4910 PRINT"OPACITY DATA ENTRY PAGE 1"
4920 PRINT STRING$(63,"=")
4930 PRINT USING P1$;MR
4940 PRINT USING P2$;MI
4950 PRINT USING P3$;L
4960 PRINT USING P4$;M
4970 PRINT USING P5$;P
4980 PRINT USING P6$;S
4982 PRINT USING P7$;DG
4984 PRINT USING P8$;SG
4990 PRINT STRING$(63,"=")
5000 PRINT @832,CHR$(91);CHR$(92);"ARE ACTIVE";
5010 PRINT @896,"USE x TO INITIATE CALCULATIONS. USE H FOR HELP"
5020 GOSUB 4610
5030 IF DD<>0 THEN 5000 ELSE DD=1
5040 IF X$ = "x" THEN RETURN ELSE IF X$ = "H" THEN 6000: GOTO 4600
5050 GOSUB 5090
5060 IP=IP+1:IF IP>MX THEN IP=3
```

```
5070 REM
5080 GOTO 4890
5090 JP=IP-2
5100 ON JP GOTO 5110,5150,5160,5170,5180,5190,5192,5194
5110 CC=44:GOSUB 4750
5120 MR=Y
5130 CC=0
5140 RETURN
5150 CC=44:GOSUB 4750:MI=Y:CC=0:RETURN
5160 CC=44:GOSUB4750:L=Y:CC=0:RETURN
5170 CC=44:GOSUB4750:M=Y:CC=0:RETURN
5180 CC=44:GOSUB4750:P=Y:CC=0:RETURN
5190 CC=44:GOSUB 4750:S=Y:CC=0:RETURN
5192 CC = 44: GOSUB 4750: DG = Y: CC = 0: RETURN
5194 CC = 44: GOSUB 4750: SG = Y: CC = 0: RETURN
5990 REM INITIALIZATION
6000 P1$="     REAL PART OF INDEX OF REFRACTION          ##.##"
6010 P2$="     IMAGINARY PART OF INDEX OF REFRACTION     #.### I"
6020 P3$="     WAVE LENGTH OF LIGHT                       #.## MICRONS"
6030 P4$="     MASS CONCENTRATION                      ##.### GMS/MC3"
6040 P5$="     PARTICLE DENSITY                         ###.## GM/CC"
6050 P6$="     STACK DIAMETER                           ##.## METERS"
6060 P7$ = "     MASS MEAN DIAMETER                       ##.### MICRONS"
6065 P8$ = "     GEOMETRIC STD DEVIATION                  ##.###"
6070 RETURN
6080 CLS
6090 PRINT STRING$(63,"=")
6100 PRINT"OPACITY PROGRAM HELP ROUTINE"
6110 PRINT"THIS PROGRAM WILL PREDICT THE OPACITY OF A PLUME OF PARTICULATE MATTER"
6120 PRINT"DATA ENTRY IS HANDLED BY FILLING IN THE DATA FORMS DISPLAYED"
6130 PRINT"ON THE CRT. THE FIRST FORM ASKS FOR GENERAL DATA "
6140 PRINT"SUCH AS WAVE LENGTH OF LIGHT, REFRACTIVE INDEX ETC. EACH DATA"
6150 PRINT"ITEM ASKED FOR IS ASKED FOR BY NAME AND WITH THE REQUIRED UNITS"
6160 PRINT"YOU MOVE AROUND THE FORM BY PRESSING THE [ AND "";CHR$(92);" ARROWS."
6170 PRINT"AFTER YOU HAVE ENTERED A DATA ITEM, PRESS ENTER TO COMPLETE"
6180 PRINT"DATA ENTRY. WHEN YOU HAVE FILLED THE FIRST PAGE,PRESS x TO START CALCULATION"
6200 PRINT"PRESS ANY KEY TO CONTINUE"
6210 Y$ = INKEY$: IF Y$ = "" THEN 6210 ELSE IF X$="M" THEN 4890ELSE RETURN
```

APPENDIX B

PROGRAM NO. 2: HISTOGRAM OPACITY PROGRAM LISTING

```
10 REM — HISTROGRAM OPACITY PROGRAM — VERSION 1.0
15 REM THIS PROGRAM CALCULATES OPACITY FROM A HISTROGRAM PARTICLE SIZE DISTRIBUTION WITH THE MIE LIGHT SCATTERING EQUATIONS
20 REM DELETE STATEMENT  30  TO COMPILE
30 CLEAR 2000
40 CLS:PRINTSTRING$(63,"="):PRINT"OPACITY PREDICTION PROGRAM"
50 PRINT STRING$(63,"=")
51 PRINT "THIS PROGRAM WAS DEVELOPED BY "
52 PRINT "S. COHEN (METEOROLOGY RESEARCH INC.)"
53 PRINT "D. ENSOR (RESEARCH TRIANGLE INSTITUTE)"
54 PRINT "L. SPARKS( ENVIRONMENTAL PROTECTION AGENCY)"
55 PRINT "EPA PROJECT OFFICER - L. SPARKS  - GRANT #R806718010"
56 PRINT" PRESS ANY KEY TO CONTINUE"
57 Y$ = INKEY$: IF Y$ = "" THEN 57
60 REM PROGRAM TO CALCULATE OPACITY WITH MIE EQUATIONS FOR HISTOGRAM SIZE
62 DIM D!(Z7),F(Z7),X(Z7),Y(Z7)
70 REM  DISTRIBUTION DATA INPUT (PROGRAM #2).
80 REM PROGRAM ASSEMBLED BY S. COHEN, ATMOSPHERIC RESEARCH GROUP 11/18/80
84 REM PROGRAM MODIFIED BY L. SPARKS FEB 1981
86 REM PROGRAM MODIFIED BY D. ENSOR JULY 1981
90 REM PROJECT OFFICER-L.E.SPARKS; ENVIRONMENTAL PROTECTION AGENCY COOPERATIVE AGREEMENT  #R806718010
99 DIM DM(13)
100 DIM R$(3)
101 DIM M2(Z7),BL(Z7),DD(Z7),C(Z7)
102 DIM S2(Z7),S3(Z7),H(Z7),DL(Z7)
104 DIM MR(56),MI(56),AR(56),AI(56),ER(56),EI(56),FR(56),FI(56)
105 DIM EX(Z7),VO(Z7),XU(Z7)
110 REM  DEFINE VARIABLES AND ARRAYS
120 DEFINT N
130 CLS: PRINT STRING$(64,"=")
132 PRINT "DO YOU WANT TO RUN SAMPLE CALCULTION? Y OR N"
134 PRINT STRING$(64,"=")
135 Y$ =INKEY$: IF Y$ ="" THEN 135 ELSE IF Y$ = "N" THEN 380 ELSE IF Y$ ="Y" THEN 140 ELSE PRINT "ANSWER Y OR N":GOTO 135
140 REM ENTER DEFAULT VALUES
150 MR = 1.5: MI = 0.0: L! =.55: P! =2.4: S = 5.0: NZ = 11: M!=.01
160 FOR IZ = 1 TO NZ
170 READ D!(IZ),F!(IZ)
180 NEXT IZ
190 DATA .2,.0101184,.4,.0930961,.5,.158655,.7,.383426
200 DATA 1.0,.5,1.5,.720713,2.0,.841345,2.5,.906904
210 DATA 4.0,.97725,7.0,.997504,10.0,.999355
300 REM MR 'REAL PART OF INDEX OF REFRACTION
310 REM MI 'IMAGINARY PART OF INDEX OF REFRACTION
320 REM  L!     'WAVELENGTH OF LIGHT (MICRONS)
330 REM  M!     'MASS CONCENTRATION (GMS / CUBIC METER)
340 REM  P!     'PARTICLE DENSITY (GMS/ CC)
350 REM  S!     'STACK DIAMETER (METERS)
360 REM  NZ     'NO. OF INPUT DATA VALUES
370 REM
380 PE!=3.141593
390 IP!=1.0/PE!
400 LT=LOG(10.0)
410 REM
420 GOSUB 6080: ' GET HELP SUBROUTINE
430 CLS:PRINT STRING$(64,"=")
440 PRINT "DO YOU WANT LINE PRINTER OUTPUT?TYPE Y OR N."
450 PRINT :PRINT STRING$(64,"=")
460 Y$=INKEY$:IFY$="" THEN 460 ELSE IF Y$="Y" THEN A$="YES" ELSE IF Y$="N" THEN A$="NO" ELSE PRINT "ANSWER Y OR N":GOTO 460
470 IF A$="YES" THEN PP%=99:GOTO 510
480 IF A$ = "NO"  THEN PP% = 0 : GOTO 510
490 PRINT "CANNOT RECOGNIZE INPUT - TRY AGAIN"
500 GOTO 440
510 REM
520 CLS
525 IF PP% = 0 THEN 570
```

```
530 CLS:PRINT STRING$(63,"="):PRINT"YOU MAY ENTER UP TO THREE LINES OF COMMENTS"
540 PRINT"ENTER COMMENTS AND PRESS ENTER AFTER EACH LINE"
550 PRINT STRING$(63,"=")
560 FOR I = 1 TO 3: LINE INPUT R$(I): IF PPZ<>0 THEN LPRINT    R$(I): NEXT I
570 GOSUB 5990
580 GOSUB 4600
590 REM
600 IF PPZ <> 0 THEN LPRINT "STACK OPACITY CALCULATION"
610 IF PPZ<>0 THEN LPRINT"INDEX OF REFRACTION=",MR,"-",MI,"xI"
620 IF PPZ <> 0 THEN LPRINT "WAVELENGTH =", L!
630 IF PPZ <> 0 THEN LPRINT "MASS CONCENTRATION =", M!
640 IF PPZ <> 0 THEN LPRINT "PARTICLE DENSITY =", P!
650 IF PPZ <> 0 THEN LPRINT "STACK DIAMETER =", S!
660 CLS
661 NZ = 0
662 FOR IX = 1 TO 27
664 IF D(IX) <> 0  THEN NZ = NZ + 1
666 NEXT IX
670 REM
680 REM CHECK CUMULATIVE FRACTIONAL DISTRIBUTION
690 FOR IX = 1 TO NZ
700 IF F(NZ) >= 1.0 THEN 3900
720 NEXT IX
730 IF PPZ <> 0 THEN LPRINT " N    PARTICLE DIAMETER   CUMULATIVE MASS"
740 IF PPZ <> 0 THEN LPRINT "        (MICROMETERS)       FRACTION"
760 FOR IX = 1 TO NZ
780 REM
800 REM
810 IF PPZ <> 0 THEN LPRINT USING "##         ###.##             .####";IX;D(IX);F(IX)
830 NEXT IX
835 GOTO 1306
840 REM
850 REM SUBROUTINE - TRAPEZOID INTEGRATION
860 REM
870 FRZ = 0
880 T1! = 0.0: T2! = 0.0: T3! = 0.0
890 I1! = 0.0: L1! = 0.0: I2! = 0.0
900 L2! =0.0: XL! = 0.0: XD! = 0.0
910       FOR DP! = D1! TO (1.01 * D2!) STEP (D2!-D1!)/10.0
920 REM     CALCULATE INTEGRANDS
930         GOSUB 1330: 'GET NUMBER DISTRIBUTION N(DP)
940         GOSUB 1390: 'GET EXTINCTION EFFICIENCY  Q
950        Z1 = DP * DP * XD
960         I1 = Z1 * Q
970         I2 = Z1 * DP
980           IF FRZ = 0 THEN 1030
990         DT = 0.5 * LOG(DP/DX) /LT
1000        T1 = T1 +(I1 + L1) * DT
1010        T2 = T2 +(I2 + L2) * DT
1020       T3 = T3 + (XD +XL) * DT
1030       DX =DP: L1 =I1: L2=I2:XL=XD:FRZ=99
1040      NEXT DP!
1050      RETURN
1060 REM
1070 REM SUBROUTINE - LEAST SQUARES FIT - Y = A + BX
1080 REM
1090 XNZ = 0: SX! = 0.0: SY! = 0.0: XY! = 0.0: XX! =0.0: YY! =0.0
1100      FOR IX = 1 TO NZ
1110       SX = SX + X(IX)
1120       SY = SY + Y(IX)
1130       XY = XY + X(IX) * Y(IX)
1140       XX = XX + X(IX) * X(IX)
1150       YY = YY + Y(IX) * Y(IX)
1160       XNZ = XNZ + 1
1170      NEXT IX
```

```
1180 REM
1190 B! = (XN% * XY - SX * SY) / (XN% * XX - SX * SX)
1200 A! = (XX  * SY - SX * XY) / (XN% * XX - SX * SX)
1210 R! = SQR(B! * ((XN% * XY -SX * SY) / (XN% * YY - SY * SY)))
1220 D5 = 10^(-A! / B!)
1230 SG = 10^(1.0 / B!)
1240 IF PP% <> 0 THEN LPRINT "MASS MEDIAN DIAMETER = ",D5
1250 IF PP% <> 0 THEN LPRINT "GEOMETRIC  STD  DEV  = ",SG
1260 IF PP% <> 0 THEN LPRINT "LOGNORMAL FIT PARAMETER = ",R!
1262 PRINT "MASS MEAN DIAMETER=",D5
1264 PRINT "GEOMETRIC STD DEV =",SG
1266 PRINT "LOGNORMAL CURVE FIT=",R!
1270 RETURN
1306 GOSUB 3280:'LOG NORMAL TRANSFORMATION OF SIZE DATA
1307 REM
1308 REM  CONTROLLING LOOP: RHOMBERG INTEGRATION OF SPLINE FIT
1309 FL% = 0: V1! = 0: V2! = 0: V3! = 0: KD% = 0
1310 REM EXTRAPOLATION BELOW D(1)
1311 D1! = .01:  D2!=D!(1)
1312 GOSUB 3002:'GET INTEGRAND PLUS INTERMEDIATE OUTPUT
1313 REM INTERPOLATION OF HISTOGRAM DATA
1314 FOR NN%=1 TO NZ-1
1315 D1!=D!(NN%):D2!=D!(NN%+1)
1316 GOSUB 3002:'GET INTEGRAND PLUS INTERMEDIATE OUTPUT
1317 NEXT NN%
1318 REM EXTRAPOLATION ABOVE D(NZ)
1319 D1!=D(NZ): D2!=100.
1320 GOSUB 3002:'GET INTEGRAND PLUS INTERMEDIATE OUTPUT
1321 GOTO 4210:' COMPUTE END RESULSTS,EG.OPACITY
1338 XI=DP!:XX=LOG(XI)/LT:IX=1:IF XX=X(1) GOTO 1355:REM SUBROUTINE SPLINE FIT INTERPOLATION
1339 IF XX=X(NZ) GOTO 1353
1340 IF XX < X(1) THEN H1 = X(1) - XX:  GOTO 1345
1341 IF XX>X(NX) GOTO 1348
1342 IX=IX+1:IF XX=X(IX) GOTO 1355
1343 IF XX>X(IX) GOTO 1342
1344 GOTO 1354: REM NEXT LINE BEGINS EXTRAPOLATION BELOW X(1)
1345 S1 = DL(1) - H(1) /(H(1) + H(2)) * 2. * (DL(2) - DL(1))
1346 YY=Y(1)+(XX-X(1))*S1:Y1=S1:GOTO 1362
1347 REM EXTRAPOLATE ABOVE X(N)
1348 S1 = DL(NZ - 1) + H(NZ - 1) * S2(NZ - 1)
1349 YY=Y(NZ)+(XX-X(NZ))*S1
1350 Y1=S1
1351 GOTO 1362
1352 REM INTERPOLATE BETWEEN X(1) &X(N)
1353 IX=NX
1354 IX=IX-1
1355 H1 = XX - X(IX): H2 = XX - X (IX + 1)
1357 PR=H1*H2
1358 Y2=S2(IX)+H1*S3(IX)
1359 DQ=(S2(IX)+S2(IX+1)+Y2)/6
1360 YY=Y(IX)+H1*DL(IX)+PR*DQ
1361 Y1=DL(IX)+(H1+H2)*DQ+PR*S3(IX)/6
1362 DG=EXP(-YY*YY/2)*Y1/SQR(2*PE)
1363 XD = DG * 6.0 /(PE * XI [ 3)
1364 IF XD<0 THEN XD = 0.0: PRINT "NEGATIVE N(DP) AT", DP
1365 RETURN
1370 REM
1380 REM
1390 REM SUBROUTINE TO CALCULATE THE EXACT EXTINCTION EFFICIENCY, Q , USING THE MIE EQUATIONS
1400 REM
1405 IF L! = 0.0 THEN PRINT"WAVELENGTH MUST HAVE POSITIVE VALUE SUCH AS .55;                PRESS ANY KEY TO CONTINUE"
1407 IF L! =0.0 THEN Y$ = INKEY$: IF Y$ ="" THEN 1407 ELSE 570
1410 XI! = PE! * DP! / L!
1420 IF XI > 40. THEN Q = 2.0: RETURN
1430 REM USE A VALUE OF 2.0 FOR Q FOR LARGE XI
1440 SM! = 0.0
```

```
1460  IF N1Z < 3 THEN N1Z = 3
1470  N1Z = N1Z + 2: 'INCLUDE 0 AND -1 SUBSCRIPTS
1480 MR!(1) = COS (XI): MI!(1) = - SIN(XI)
1485 MR!(2) = SIN (XI): MI!(2) = COS(XI)
1490 REM CALCULATE THE  A(N)
1500 PP! = MR * XI: QQ! = MI * XI
1510 REM SINH(Q) AND COSH(Q)
1520 TT! = EXP(QQ!)
1530 SH! = (TT - 1.0 / TT) * .5
1540 CH! = (TT + 1.0 / TT) * .5
1550 T4! = SIN (PP): T5! = T4 * T4 + SH * SH
1560 AR!(2) = T4! * COS (PP) / T5:  AI!(2) = SH * CH / T5
1570     FOR IZ = 3 TO N1Z
1580       I1Z = IZ - 1:  IZZ = IZ - 2
1590       PR! = (2 * IZZ - 1) / XI
1600       MR(IZ) = PR * MR(I1Z) - MR(IZZ)
1610       MI(IZ) = PR * MI(I1Z) - MI(IZZ)
1620       PR = IZZ / XI: TT = MR * MR + MI * MI
1630       QI = (PR * MI) / TT: QR = (PR * MR) /TT
1640       PR = QR - AR(I1Z):   PI = QI - AI(I1Z)
1650       TT = PR * PR + PI * PI
1660      AR(IZ) = PR / TT - QR: AI(IZ) = -PI / TT - QI
1670       Y1 = ABS (ER(I1Z)) + ABS (EI(I1Z))
1680         IF IZ > 3 AND Y1 < 1.0 E-20 THEN ER(IZ) = 0.0:    EI(IZ) = 0.0 : GOTO 1760
1690            TT = MR * MR + MI * MI
1700            TI = (AI(IZ) * MR + AR(IZ) * MI) /TT
1710            TR = (AR(IZ) * MR - AI(IZ) * MI) / TT +IZZ / XI
1720            PR = TR * MR(IZ) - MR(I1Z): PI = TI *MR(IZ)
1730            QR = TR * MR(IZ) - TI * MI(IZ) - MR(I1Z): QI = TR * MI(IZ) + TI * MR(IZ) - MI(I1Z)
1740            TT = QR * QR + QI * QI
1750            EI(IZ) = (PI * QR - PR * QI) / TT: ER(IZ) = (PR* QR + PI * QI)/ TT
1760       Y1 = ABS (FR!(I1Z)) + ABS ( FI!(I1Z))
1770       IF IZ > 3  AND Y1 < 1.0 E -20 THEN FR(IZ) = 0.0: FI(IZ) = 0.0 :GOTO 1850
1780            TI = MR * AI(IZ) - MI * AR(IZ)
1790            TR = MR * AR(IZ) + MI * AI(IZ) + IZZ / XI
1800            UR = TR * MR(IZ) - MR(I1Z): UI = TI * MR(IZ)
1810            PI = TR * MI(IZ) + TI * MR(IZ) - MI(I1Z)
1820            QR = TR * MR(IZ) - TI * MI(IZ) - MR(I1Z)
1830            TT = QR * QR + PI * PI
1840            FR(IZ) = (UR * QR + UI * PI) / TT: FI(IZ) =          (UI * QR - UR * PI) / TT
1850       SH = SH + (2 * IZZ + 1) * (ER(IZ) + FR(IZ))
1860       NEXT IZ
1870      Q = 2.0 * SH / (XI * XI)
1880  PRINT "DIAM = ",DP,"Q = ",Q
1890 PRINT "N(DP)=",XO
1900 RETURN
3002 '  PPZ<>0 THEN LPRINT"LOWER-UPPER DIAMETER",D1,"-",D2
3004 PRINT "LOWER-UPPER DIAMETER",D1,"-",D2
3013 GOSUB 850: 'CALCULATE THE INTEGRAND
3014 V1! = V1! + T1!: V2! = V2! + T2!: V3! = V3! + T3!
3015 IF PPZ <> 0 THEN LPRINT"EXTINCTION"," VOLUME  "," NUMBER  "
3016 IF PPZ <> 0 THEN LPRINT USING"##.####^^^^       ";T1!,T2!,T3!
3017 PRINT "EXTINCTION","VOLUME","NUMBER"
3018 PRINT T1,T2,T3: KDZ =KDZ + 1: EX(KDZ) = T1: VO(KDZ) = T2: XU(KDZ) = T3
3019 RETURN
3280 REM<<<xxxSUBROUTINE NORMAL TRANSFORMATIONxxx>>>
3290 C0=2.515517
3300 C1=0.802853
3310 C2=0.010328
3320 D1=1.432788
3330 D2=0.189269
3340 D3=0.001308
3350 LT=LOG(10.0)
3360 KZ=0
3370 FOR IZ=1 TO NZ
3380 KZ=KZ+1
```

```
3381 X(KZ)=LOG(D(II))/LT
3382 CU = F(II)
3385 PLX=1
3395 IF CU<=.5 GOTO 3410
3397 PLX=-1
3400 CU=1-CU
3410 T=SQR(-2*LOG(CU))
3420 Y(KZ)=(-T+(C0+C1*T+C2*T*T)/(1+T*(D1+T*(D2+T*D3))))*PLX
3430 NEXT II
3460 FOR II=1 TO NZ/2
3470 TX=X(II):TY=Y(II)
3480 X(II)=X(NZ+1-II):Y(II)=Y(NZ+1-II)
3490 X(NZ+1-II)=TX:Y(NZ+1-II)=TY
3500 NEXT II
3510 FOR II=1 TO NZ-1
3520 FOR JJ=II+1 TO NZ
3530 IF X(JJ)>=X(II) GOTO 3570
3540 TX=X(II):TY=Y(II)
3550 X(II)=X(JJ):Y(II)=Y(JJ)
3560 X(JJ)=TX:Y(JJ)=TY
3570 NEXT JJ
3580 NEXT II
3590 GOSUB 1070: ' COMPUTE LOGNORMAL FIT OF PARTICLE SIZE DATA
3592 IF SG < 1. THEN PRINT "*** WARNING *** GEOMETRIC STANDARD DEVIATION < 1;IE PHYSICALLY IMPOSSIBLE SIZE MEASUREMENTS.          PR
ESS ANY KEY TO CONTINUE.
3594 IF SG < 1. THEN Y$ = INKEY$: IF Y$="" THEN 3594 ELSE 570
3596 IF SG >10. OR D5 > 100. OR D5 < .01 THEN PRINT "PARTICLE  SIZE DISTRIBUTION IS OUT OF RANGE FOR THIS PROGRAM.
PRESS ANY KEY TO CONTINUE."
3598 IF SG> 10. OR D5 > 100. OR D5 < .01 THEN Y$ = INKEY$: IF   Y$ = "" THEN 3598 ELSE 570
3600 REM <<<***SPLINE FIT***>>>
3610 OM=1.0717968: REM 'RELAXATION PARAMETER
3620 VT=SQR(6.2832)
3630 REM -FIRST DIFFERENCES
3640 FOR I=1 TO NZ-1
3650 H(I)=X(I+1)-X(I)
3660 DL(I)=(Y(I+1)-Y(I))/H(I)
3670 NEXT I
3680 REM -SECOND DIFFERENCES
3690 FOR I=2 TO NZ-1
3700 H2(I)=H(I-1)+H(I)
3710 BL(I)=.5*H(I-1)/H2(I)
3720 DQ(I)=(DL(I)-DL(I-1))/H2(I)
3730 S2(I)=2*DQ(I)
3740 C(I)=3*DQ(I)
3750 NEXT I
3760 S2(1)=0
3770 S2(NZ)=0
3780 REM SUCCESSIVE OVER-RELAXATION SOLUTION
3790 ET=0
3800 FOR I=2 TO NZ-1
3810 W=(C(I)-BL(I)*S2(I-1)-(.5-BL(I))*S2(I+1)-S2(I))*OM
3820 IF ABS(W)>ET THEN ET=ABS(W)
3830 S2(I)=S2(I)+W
3840 NEXT I
3850 IF ET>1E-5 GOTO 3790
3860 REM THIRD DIFFERENCES
3870 FOR I=1 TO NZ-1
3880 S3(I)=(S2(I+1)-S2(I))/H(I)
3890 NEXT I
3892 RETURN
3900 REM
3910 REM  NORMALIZE CUMULATIVE DISTRIBUTION IF
3920 REM   REQUIRED; IE. IF CU > 1.0
3930    FOR II = 1 TO NZ
3940 F(II) = F(II)/ F(NZ)
3950    NEXT II
```

```
3960 F(NZ) = 0.0: D(NZ) = 0.0
3970 NZ = NZ - 1
3980 GOTO 680
4210  PRINT "INTEGRALS =", V1, V2, V3
4220 IF PP%<> 0 THEN LPRINT "INTEGRALS( EXTINCTION, VOLUME,NUMBER,) =",V1,V2,V3
4230      FOR IX = 1 TO NZ + 1
4240        EX(IX) = EX(IX) / V1 * 100.
4250       VO(IX) = VO(IX)/ V2 * 100.
4260       XU(IX) = XU(IX) / V3 * 100.
4270     NEXT IX
4345 IF EX(1) OR EX(NZ +1) > 90. THEN PRINT "PRESS ANY KEY TO  OBTAIN FINAL RESUTLS":
4347 IF EX(1) OR EX (NZ +1) > 90. THEN Y$ = INKEY$:IF Y$ =""   THEN 4347
4350 IF PP% <> 0 THEN LPRINT"LOWER - UPPER DIAMETER","%EXTINCTION      %VOLUME         %NUMBER"
4360 IF PP% <> 0 THEN LPRINT".01",D(1),EX(1),VO(1),XU(1)
4370 FOR IX = 2 TO NZ
4380 IF PP% <> 0 THEN LPRINT D(IX - 1),D(IX),EX(IX),VO(IX),XU(IX)
4390      NEXT IX
4400 IF PP% <> 0 THEN LPRINT D(NZ),"100",EX(NZ + 1),VO(NZ + 1),XU(NZ + 1)
4410 IF EX(1) > 50. OR EX(NZ + 1) > 50. AND PP% <> 0 THEN LPRINT"***** WARNING ***** MORE THAN 50 PERCENT OF THE LIGHT EXTINCTION":
IF PP% <> 0 THEN LPRINT"OCCURS OUTSIDE THE MEASURED PARTICLE SIZE RANGE."
4415 IF EX(1) > 50. OR EX(NZ + 1) > 50. THEN PRINT"******** WARNING ******** MORE THAN 50 PERCENT OF THE LIGHT         EXTINCTION OCCU
RS OUTSIDE THE MEASURED PARTICLE SIZE RANGE."
4420 REM PRINT "INTEGRALS=",V1,V2,V3
4422 SP = 1.5 * V1/V2
4424 OP = 100. * (1. - EXP(-SP * M * S / P))
4430 PRINT""
4435 PRINT "MASS MEAN DIAMETER =",DS
4437 PRINT "GEOMETRIC STD DEV =",SG
4438 PRINT "LOGNORMAL CURVE FIT =",R!
4440 PRINT "SPECIFIC EXTINCTION COEFFICIENT=",SP
4450 PRINT"MASS CONCENTRATION=",M
4460 PRINT"PARTICLE DENSITY=",P
4470 PRINT "STACK DIAMETER=",S
4480 PRINT "OPACITY(%)=",OP
4490 IF PP% <> 0 THEN LPRINT "SPECIFIC EXTINCTION COEFFICIENT  (M2/CM3) = ", SP
4500 IF PP% <> 0 THEN LPRINT " OPACITY(%) =", OP
4550 PRINT "DO YOU WANT TO RUN ANOTHER CASE? Y OR N"
4560 Y$=INKEY$: IF Y$="" THEN 4560 ELSE IF Y$ ="N" THEN END    ELSE IF Y$="Y" THEN 570 ELSE PRINT "ANSWER Y OR N": GOTO 4560
4600 MX=8:IP=3:GOSUB 4890
4610 REM *** POINTER CONTROL FOR MENUES ***
4620 PRINT @IP%64,CHR$(94);
4630 GOSUB 4710
4640 PRINT @IP%64," ";
4650 DD=0
4660 IF X=27 OR X=91 THEN DD=-1
4670 IF X=26 OR X=10 OR X=13 THEN DD=+1
4680 IP=IP+DD : IF IP <1 THEN IP=MX
4690 IF IP>MX THEN IP=3
4700 RETURN
4710 REM *** GET AN UNSHIFTED CHARACTER FROM KEYBOARD ***
4720 X$=INKEY$ : IF X$="" THEN 4720 ELSE X=ASC(X$)
4725 IF X$="x" THEN 600
4730 IF X>95 THEN X=X-32 : X$=CHR$(X)
4740 RETURN
4750 REM *** NUMERIC PARAMETER INPUT USING SUBR @ 1900
4760 PRINT @IP%64+CC,STRING$(7," ");
4770 GOSUB 4790 : Y=VAL(Y$)
4780 RETURN
4790 REM *** STRING INPUT, ADDING TO Y$ STARTING WITH X$ ***
4800 CC=CC+1
4810 Y$=X$
4820 PRINT @IP%64+CC,Y$;CHR$(95);" ";
4830 GOSUB 4710
4840   IF X=13 THEN CC=CC-1 : RETURN
4850   IF X=8 THEN IF LEN(Y$)>0 THEN Y$=LEFT$(Y$,LEN(Y$)-1)
4860   IF X=24 THEN Y$=""
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4870   IF X>31 THEN Y$=Y$+X$
4880 GOTO 4820
4890 CLS
4895 MX = 8: IF IP < 3 THEN IP = 8
4900 PRINT STRING$(63,"=")
4910 PRINT"OPACITY DATA ENTRY PAGE 1"
4920 PRINT STRING$(63,"=")
4930 PRINT USING P1$;MR
4940 PRINT USING P2$;MI
4950 PRINT USING P3$;L
4960 PRINT USING P4$;M
4970 PRINT USING P5$;P
4980 PRINT USING P6$;S
4990 PRINT STRING$(63,"=")
5000 PRINT @704,CHR$(91);CHR$(92);" ARE ACTIVE USE > TO GO TO NEXT PAGE";
5010 PRINT@768,"USE x TO INITIATE CALCULATIONS. USE H FOR HELP"
5020 GOSUB 4610
5030 IF DD<>0 THEN 5080 ELSE DD=1
5040 IF X$="x" THEN RETURN ELSE IF X$=">" THEN 5200 ELSE IF X$="H" THEN GOSUB 6000:GOTO4600
5050 GOSUB 5090
5060 IP=IP+1:IF IP>MX THEN IP=3
5070 GOTO 4890
5080 GOTO 4890
5090 JP=IP-2
5100 ON JP GOTO 5110,5150,5160,5170,5180,5190
5110 CC=44:GOSUB 4750
5120 MR=Y
5130 CC=0
5140 RETURN
5150 CC=44:GOSUB 4750:MI=Y:CC=0:RETURN
5160 CC=44:GOSUB4750:L=Y:CC=0:RETURN
5170 CC=44:GOSUB4750:M=Y:CC=0:RETURN
5180 CC=44:GOSUB4750:P=Y:CC=0:RETURN
5181 SX  = 0.0
5182 SY  = 0.0
5183 XY  = 0.0
5184 XX  = 0.0
5185 YY  = 0.0
5190 CC=44:GOSUB 4750:S=Y:CC=0:RETURN
5200 REM PARTICLE SIZE DISTRIBUTION INPUT
5210 JS=1:MX=10:JL=10:IL=2
5220 CLS
5230 PRINT "ENTER PARTICLE SIZE DISTRIBUTION"
5240 PRINT "AS A CUMULATIVE MASS"
5250 PRINT "FRACTION LESS THAN."
5255 PRINT "START WITH SMALLEST PARTICLE DIAMETER! "
5257 PRINT "THE CUMULATIVE MASS FRACTIONS MUST INCREASE"
5258 PRINT " FROM SMALLEST TO LARGEST DIAMETERS!"
5260 PRINT "PRESS ANY KEY TO CONTINUE"
5270 Y$ = INKEY$: IF Y$ = "" THEN 5270
5350 IP=IL
5360 CLS
5370 PRINT STRING$(63,"=")
5380 PRINT"I     DIAMETER MICRONS          CUMULATIVE MASS(<)";Y1$
5390 J = JS: JL = JS + 8
5395 IF JS>19 THEN JS=19: JL=27
5400 IF MX<JL THEN MX=JL
5410 FOR J=JS TO JL
5420 PRINT   J;"      ";D(J);TAB(40);F(J)
5430 NEXT J
5440 PRINT @768,STRING$(31,95);
5450 PRINT@832, CHR$(91);CHR$(92);CHR$(93);CHR$(94);" ARE ACTIVE USE x TO START CALCULATIONS";
5460 PRINT@896,"USE > TO GO TO NEXT PAGE < TO GO TO PREVIOUS PAGE";
5470 GOSUB 5680 :REM POINTER CONTROL
5480 IF ID<> 0 THEN 5640 ELSE ID=1
5490 IF X=62 OR X=60 OR X$="x" THEN 5590
```

```
5500 JP=IP-IL+1
5510 GOSUB 5850
5520 IF IC = 9 THEN D(JP+JS-1) = Y
5530 IF JP+JS-1>N THEN N=JP+JS-1
5540 IF IC=34 THEN F(JP+JS-1)=Y
5550 IF IC = 9 THEN IC = 34: GOTO 5360
5560 IF IC = 34 THEN IC = 9
5570 IP=IP+1
5580 GOTO 5360
5590 IF X = 62 THEN JS=JL + 1: IC = 9: GOTO 5350
5600 IF X<>60 THEN 5630 ELSE JS=JS-9
5605 IF JS< 1 THEN JS = 1 :IP =3: GOTO 4090
5610 IF JS<1 THEN JS=1
5620 IC = 9: GOTO 5350
5630 IF X$="x" THEN 600 ELSE 5640
5640 PRINT@IP%64+IC," ";
5650 IF IP>MX THEN IP=IL
5660 PRINT @IP%64+IC,CHR$(94);
5670 GOTO5470
5680 REM xxx POINTER CONTROL FOR MENUES xxx
5685 IF IC = 0 THEN IC = 9
5690 PRINT @IP%64+IC,CHR$(94);
5700 GOSUB 5810
5710 PRINT @IP%64+IC," ";
5720 ID=0
5730 IF X=27 OR X=91 THEN ID=-1
5740 IF X=26 OR X=10 OR X=13 THEN ID=+1
5750 IP=IP+ID : IF IP<IL THEN IP=MX
5760 IF IP>MX THEN IP=IL
5770 IF X = 8 THEN IC = 9
5780 IF X =9 THEN IC =34
5790 IF X=8 OR X=9 THEN ID=1
5800 RETURN
5810 REM xxx GET AN UNSHIFTED CHARACTER FROM KEYBOARD xxx
5820 X$=INKEY$ : IF X$="" THEN 5820 ELSE X=ASC(X$)
5830 IF X>95 THEN X=X-32 : X$=CHR$(X)
5840 RETURN
5850 REM xxx NUMERIC PARAMETER INPUT USING SUBR @ 1900
5860 PRINT @IP%64+IC,STRING$(4," ");
5870 GOSUB 5890 : Y=VAL(Y$)
5880 RETURN
5890 REM xxx STRING INPUT, ADDING TO Y$ STARTING WITH X$ xxx
5900 CC=CC+1
5910 Y$=X$
5920 PRINT @IP%64+IC,Y$;CHR$(95);" ";
5930 GOSUB 5810
5940   IF X=13 THEN CC=CC-1 : RETURN
5950   IF X=8 THEN IF LEN(Y$)>0 THEN Y$=LEFT$(Y$,LEN(Y$)-1)
5960   IF X=24 THEN Y$=""
5970   IF X>31 THEN Y$=Y$+X$
5980 GOTO 5920
5990 REM INITIALIZATION
6000 P1$="     REAL PART OF INDEX OF REFRACTION          ##.##"
6010 P2$="     IMAGINARY PART OF INDEX OF REFRACTION     #.### I"
6020 P3$="     WAVE LENGTH OF LIGHT                       #.## MICRONS"
6030 P4$="     MASS CONCENTRATION                       ##.### GMS/MC3"
6040 P5$="     PARTICLE DENSITY                          ###.## GM/CC"
6050 P6$="     STACK DIAMETER                            ##.## METERS"
6060 P7$="PARTICE DIAMETER ##.## MICRONS"
6070 RETURN
6080 CLS
6090 PRINT STRING$(63,"=")
6100 PRINT"OPACITY PROGRAM HELP ROUTINE"
6110 PRINT"THIS PROGRAM WILL PREDICT THE OPACITY OF A PLUME OF PARTICULATE MATTER"
6120 PRINT"DATA ENTRY IS HANDLED BY FILLING IN THE DATA FORMS DISPLAYED"
6130 PRINT"ON THE CRT. THE FIRST FORM ASKS FOR GENERAL DATA "
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6140 PRINT"SUCH AS WAVE LENGTH OF LIGHT, REFRACTIVE INDEX ETC. EACH DATA"
6150 PRINT"ITEM ASKED FOR IS ASKED FOR BY NAME AND WITH THE REQUIRED UNITS"
6160 PRINT"YOU MOVE AROUND THE FORM BY PRESSING THE [ AND "";CHR$(92);" ARROWS."
6170 PRINT"AFTER YOU HAVE ENTERED A DATA ITEM, PRESS ENTER TO COMPLETE"
6180 PRINT"DATA ENTRY. WHEN YOU HAVE FILLED THE FIRST PAGE,PRESS > TO "
6190 PRINT"GO TO THE SECOND PAGE."
6200 PRINT"PRESS ANY KEY TO CONTINUE."
6210 Y$=INKEY$:IF Y$="" THEN 6210
6220 CLS
6230 PRINT STRING$(63,"=")
6240 PRINT"THE REMAINING PAGES ARE USED FOR THE PARTICLE SIZE DISTRIBUTION"
6250 PRINT"THE PARTICLE SIZE DISTRIBUTION MAY BE ENTERED ONLY AS"
6260 PRINT"A CUMULATIVE MASS FRACTION LESS THAN. CONTROL"
6270 PRINT"MOVEMENT AROUND THE PARTICLE SIZE DISTRIBUTIONS FORMS USING"
6280 PRINT"THE FOUR ARROWS. TO CHANGE PAGES USE < OR >. WHEN ALL"
6290 PRINT"THE DATA ENTERED ARE CORRECT, PRESS x TO BEGIN CALCULA-"
6300 PRINT"TIONS. PRESS ANY KEY TO CONTINUE.
6320 Y$ =INKEY$: IF Y$ = "" THEN 6320 ELSE RETURN
```